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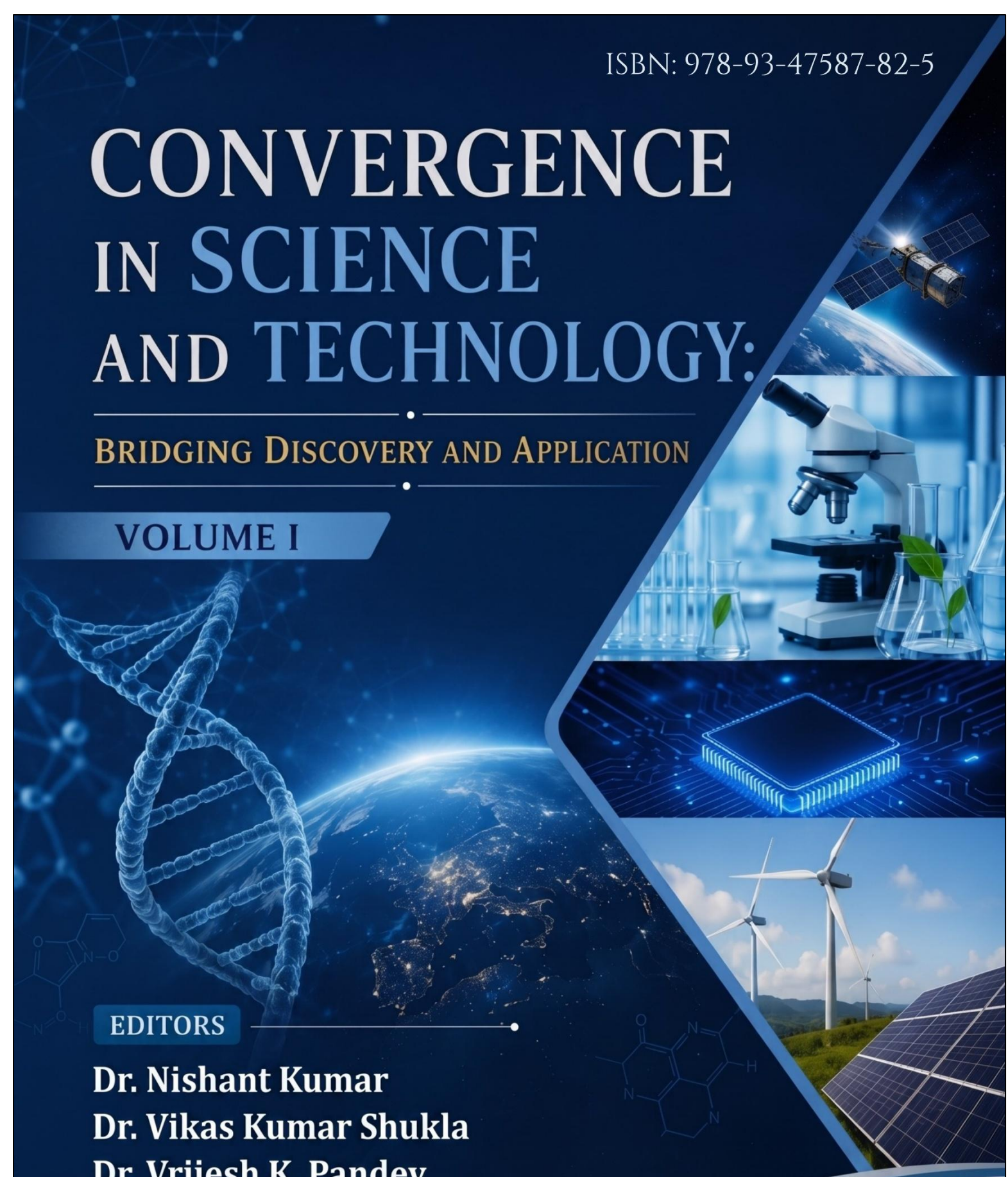
CONVERGENCE IN SCIENCE AND TECHNOLOGY:

BRIDGING DISCOVERY AND APPLICATION

VOLUME I



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Convergence in Science and Technology: Bridging Discovery and Application

Volume I

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PREFACE

Science and technology have transformed the modern world by expanding the boundaries of knowledge, accelerating innovation, and creating solutions to complex societal challenges. In the contemporary era, meaningful progress increasingly depends on the convergence of diverse scientific disciplines with emerging technologies and their practical applications. Convergence in Science and Technology: Bridging Discovery and Application has been conceived with this perspective to present a broad and interdisciplinary platform for sharing recent developments, innovative ideas, research findings, and practical approaches across science and technology.

The book brings together contributions that demonstrate how fundamental scientific discoveries can be translated into useful technologies, sustainable practices, and socially relevant applications. It emphasizes the interconnected nature of disciplines such as biological sciences, environmental science, physical sciences, chemistry, agriculture, information technology, engineering, and emerging technological domains. Such interdisciplinary interactions are essential for addressing contemporary issues including climate change, environmental degradation, food and nutritional security, biodiversity conservation, sustainable development, public health, and technological advancement.

A central objective of this volume is to encourage researchers, academicians, teachers, students, and professionals to look beyond disciplinary boundaries and recognize opportunities for collaboration. The chapters included in this book reflect the importance of integrating scientific knowledge with innovation, technology, and real-world problem solving. They also highlight the role of research and education in developing sustainable and inclusive solutions for society.

We hope that this volume will serve as a valuable reference for students, teachers, researchers, and practitioners seeking to understand emerging trends and interdisciplinary approaches in science and technology. It is our sincere belief that the convergence of discovery and application will continue to inspire new ideas, strengthen collaborative research, and contribute meaningfully to a sustainable and technologically advanced future.

The editors gratefully acknowledge the valuable contributions of all authors and reviewers whose efforts have made this volume possible.

- Editors

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NODES OF TRUST: GRAPH-THEORETIC FOUNDATIONS FOR NEXT-GENERATION CRYPTOGRAPHIC SECURITY

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Abstract

Graph theory and cryptography have evolved along parallel trajectories for more than a century, yet their convergence has only recently matured into a coherent and productive research programme. This chapter presents an integrated account of how graph-theoretic structures, including expander graphs, Cayley graphs, and spectral properties of adjacency and Laplacian matrices, underpin the design and analysis of contemporary cryptographic primitives. Beginning with the foundational vocabulary of graphs and classical and modern cryptography, the discussion proceeds to show how graph traversal, coloring, isomorphism, and spectral techniques are exploited to construct collision-resistant hash functions, key-exchange protocols, and post-quantum candidates whose security rests on the computational hardness of graph-theoretic problems such as finding paths in expander graphs or computing isogenies between elliptic curves. The chapter further surveys applied domains in which graph-based cryptographic reasoning has demonstrable value, including healthcare data protection, the Internet of Things, blockchain transaction analysis, cloud computing, wireless sensor networks, artificial intelligence, and broader cybersecurity operations such as intrusion detection. Emerging directions are examined, with particular attention to post-quantum cryptography, graph neural networks, AI-assisted cryptanalysis, and dynamic graph-based encryption schemes capable of adapting to evolving threat landscapes. By synthesising mathematical rigor with applied relevance, the chapter argues that graph theory offers not merely a descriptive language for cryptographic systems but a generative source of new security guarantees, positioning it as a central pillar of the discovery-to-application pipeline that defines contemporary information security research.

Keywords: Graph Theory, Cryptography, Expander Graphs, Network Security, Post-Quantum Cryptography, Graph Neural Networks, Spectral Graph Theory, Blockchain Security.

1. Introduction

Graph theory originated in 1736 with Leonhard Euler's resolution of the Königsberg bridge problem and has since matured into a discipline concerned with vertices, edges, and the structural relationships that bind them, evolving into a foundational modelling tool across

computer science, operations research, biology, and physics. Cryptography, in parallel, traces its lineage to antiquity through substitution and transposition ciphers, matured through the mechanical cipher systems of the twentieth century, and was transformed decisively by the introduction of public-key cryptography, which replaced the assumption of a shared secret with computational hardness assumptions rooted in number theory (Diffie & Hellman, 1976; Rivest *et al.,* 1978).

The integration of graph theory with cryptography reflects a deep structural affinity between the two fields. Cryptographic hardness assumptions frequently reduce to combinatorial problems on graphs, such as finding short paths, computing isomorphisms, or locating small eigenvalue gaps, all of which are naturally analysed using graph-theoretic tools. Expander graphs, Cayley graphs, and spectral graph invariants have each been shown to yield cryptographic primitives whose security proofs rely on well-studied mathematical hardness results rather than ad hoc heuristics (Lubotzky *et al.,* 1988; Charles *et al.,* 2009). This convergence is especially important in an era in which quantum computation threatens the number-theoretic assumptions underlying classical public-key cryptography, motivating a search for alternative hard problems, many of which are graph-theoretic in nature (De Feo *et al.,* 2014; National Institute of Standards and Technology, 2020).

The motivation for this chapter arises because a unified treatment connecting graph-theoretic fundamentals to cryptographic applications remains scarce for readers approaching the subject from either a mathematics or applied computer science background. Accordingly, the chapter pursues three objectives: to consolidate the essential concepts of graph theory and cryptography into a shared vocabulary; to demonstrate, with concrete examples, how specific graph structures and algorithms are deployed within cryptographic constructions; and to survey the applied domains and emerging research directions in which graph-based cryptography is expected to exert the greatest influence over the coming decade. Section 2 reviews graph-theoretic fundamentals; Section 3 summarises cryptography; Section 4 examines their intersection; Section 5 surveys applications; Section 6 discusses emerging trends; and Section 7 concludes the chapter.

2. Fundamentals of Graph Theory

A graph G = (V, E) consists of a set of vertices V and a set of edges E connecting pairs of vertices, serving as an abstraction of any system in which discrete entities interact pairwise. Graphs may be undirected or directed, and weighted when a numerical cost is associated with each edge. Structural notions such as vertex degree, connectivity, cycles, planarity, bipartiteness, and diameter each have direct analogues in the analysis of graph-based cryptographic constructions. Graphs are commonly represented through adjacency matrices, adjacency lists, or incidence matrices, and the chosen representation materially affects algorithmic efficiency, a

consideration that carries over into the computational cost of graph-based cryptographic primitives.

Certain specialised families of graphs are of particular cryptographic interest. Cayley graphs are constructed from a group and a generating set, producing highly symmetric, vertex-transitive structures suited to modelling algebraic hardness assumptions. Expander graphs are sparse yet highly connected graphs exhibiting rapid random-walk mixing, a property underlying randomness extraction and collision-resistant hashing. Spectral graph theory, which studies the eigenvalues of the adjacency or Laplacian matrix, quantifies connectivity and expansion through the spectral gap, which bounds the mixing rate and, by extension, the security margin of graph-based hash constructions (Lubotzky *et al.,* 1988).

Several algorithmic problems on graphs carry direct cryptographic relevance: shortest-path algorithms determine the practical hardness of traversal-based schemes; graph coloring, which labels vertices such that no two adjacent vertices share a label, is exploited in zero-knowledge proofs; and graph isomorphism testing, for which no known polynomial-time algorithm exists, underlies isomorphism-based identification schemes. Table 1 summarises the principal graph families and algorithms discussed alongside their cryptographic relevance.

Table 1: Graph-theoretic structures and algorithms of principal cryptographic relevance.

Graph Structure / Algorithm	Defining Property	Cryptographic Relevance
Cayley graph	Built from a group and generating set; vertex-transitive	Algebraic hardness assumptions; group-based key exchange
Expander graph	Sparse, highly connected, rapid random-walk mixing	Collision-resistant hash construction (CGL, LPS hashes)
Spectral (eigenvalue) analysis	Studies eigenvalues of adjacency / Laplacian matrix	Quantifies expansion; bounds hash security margin
Graph isomorphism testing	No known general polynomial-time algorithm	Identification and zero-knowledge protocols
Graph coloring	Vertex labelling with adjacency constraints	Zero-knowledge proofs of knowledge
Shortest-path / traversal	Determines reachability and path cost	Path-finding hardness in hash and puzzle schemes

3. Fundamentals of Cryptography

Classical cryptography, spanning substitution ciphers through to the mechanical systems of the early twentieth century, relied on the secrecy of the algorithm or key and offered limited resistance to systematic cryptanalysis once the underlying structure was understood. Modern cryptography departs from this model by embracing Kerckhoffs's principle, whereby security

depends solely on the secrecy of the key, and by grounding security claims in computational hardness assumptions that can be formally analysed. This shift enabled symmetric-key encryption, in which the same key is used for both encryption and decryption and which remains the workhorse of bulk data protection, and asymmetric or public-key encryption, introduced by Diffie and Hellman (1976) and realised concretely by Rivest *et al.* (1978) through RSA, which allows secure communication without prior key sharing by exploiting the asymmetry between easy and hard computational directions, such as multiplication versus factorisation.

Beyond encryption, modern cryptographic systems rely on hash functions, which map arbitrary-length input to fixed-length output such that inversion and collisions are computationally infeasible; digital signature schemes, which bind a message to a signer's identity and provide non-repudiation; and key-exchange protocols, which allow two parties to agree upon a shared secret over an insecure channel. The security of these primitives is typically reduced to well-studied problems, including integer factorisation, the discrete logarithm problem, and, increasingly, problems defined over graphs and lattices believed to resist quantum-capable adversaries (Menezes *et al.,* 1996; National Institute of Standards and Technology, 2020). Table 2 contrasts the principal categories of cryptographic mechanism discussed in this section.

Table 2: Core cryptographic mechanisms and their underlying computational hardness assumptions

Mechanism	Core Function	Representative Hardness Assumption
Symmetric encryption	Confidentiality using a shared secret key	Resistance to differential / linear cryptanalysis
Asymmetric encryption	Confidentiality without prior key sharing	Integer factorisation; discrete logarithm
Cryptographic hash function	Integrity and fixed-length digesting	Collision resistance; preimage resistance
Digital signature	Authentication and non-repudiation	Hardness of forging under chosen-message attack
Key exchange	Establishing a shared secret over open channels	Diffie–Hellman problem; graph path-finding hardness

4. Graph Theory in Cryptography

The most direct application of graph theory to cryptography is found in graph-based hashing schemes, in which security is reduced to a well-defined problem on a specific graph family. Charles *et al.* (2009) built collision-resistant hash functions from expander graphs, notably the Ramanujan graphs of Lubotzky *et al.* (1988) and the isogeny graphs studied by Pizer, by encoding a message as a walk whose terminal vertex constitutes the digest; collision resistance

follows from the difficulty of finding two distinct paths between the same vertex pair. Subsequent cryptanalysis showed that not all expander families offer equivalent security: Tillich and Zémor (2008) and Petit *et al.* (2008) exhibited efficient collision- and preimage-finding attacks against the Lubotzky–Phillips–Sarnak and Morgenstern constructions, underscoring that expansion alone is insufficient and that concrete algebraic structure must be scrutinised. More recent proposals, such as the Markoff-triple hash of Fuchs *et al.* (2022), continue this programme by seeking graph families combining provable expansion with resistance to known algebraic attacks.

Graph traversal underlies a second class of constructions in which path-finding hardness supports computational puzzles and proof-of-work schemes. Graph coloring finds its principal application in zero-knowledge proofs, where a prover demonstrates knowledge of a valid coloring without revealing it, providing a general template for zero-knowledge proofs of NP-complete problems. Cayley graphs, formed from a finite group and a symmetric generating set, bridge group theory and graph theory and are used both to construct expander families with provable spectral gaps and to model the state spaces of post-quantum isogeny-based schemes such as CSIDH, in which vertices correspond to isogenous elliptic curves and edges to isogenies of fixed degree (Castryck *et al.,* 2018; De Feo *et al.,* 2014).

Graph isomorphism, determining whether two graphs are structurally identical up to relabelling, is neither known to be solvable in polynomial time nor known to be NP-complete, making it attractive for identification schemes whose security does not rely on number-theoretic assumptions vulnerable to quantum attack. Spectral graph theory certifies the security of expander-based constructions: the spectral gap quantifies how rapidly a random walk mixes, and Ramanujan graphs, which achieve the optimal spectral gap, are the preferred substrate for provably secure hash functions (Lubotzky *et al.,* 1988; Costache *et al.,* 2019). Collectively, these tools offer security advantages complementing classical number-theoretic cryptography, including resistance to certain quantum algorithms, algebraic diversity that limits single-breakthrough risk, and a toolkit for zero-knowledge protocols with provable security bounds.

5. Applications

The applied reach of graph-theoretic cryptography extends across contemporary computing domains. In healthcare, patient data-sharing networks are naturally modelled as graphs connecting providers, devices, and records, and graph-based access-control and hashing schemes support tamper-evident audit trails and fine-grained authorisation while preserving privacy under regulatory constraints. In the Internet of Things, where resource-constrained devices form dense, dynamically changing topologies, graph representations of connectivity enable lightweight key-distribution and graph neural network based intrusion detection, such as the E-GraphSAGE

framework, which models network flows as edge features to identify malicious traffic with improved accuracy over flow-based baselines (Lo *et al.,* 2022).

Blockchain systems are, by construction, graph-structured: transactions form directed graphs linking addresses, and smart-contract interactions add further relational layers. Graph analysis of these networks has proven effective for detecting fraudulent schemes, including Ponzi-scheme contracts on Ethereum, by identifying anomalous topological patterns such as concentrated in-degree or characteristic fund-flow cycles (Chen *et al.,* 2018). In cloud computing, graph models of virtual machine placement and access-control hierarchies support detection of privilege-escalation paths and multi-tenant key management. Wireless sensor networks, constrained by energy and unreliable connectivity, benefit from Cayley-graph and expander-graph based key pre-distribution schemes guaranteeing network-wide connectivity with minimal stored keys per node, directly leveraging the properties discussed in Section 4.

Artificial intelligence and cybersecurity increasingly intersect with graph-based cryptography through graph neural networks, which extend deep learning to graph-structured data and have been applied to intrusion detection, malware provenance analysis, and anomaly detection across enterprise networks (Wu *et al.,* 2021). By representing traffic, authentication logs, or dependency structures as graphs, these models capture relational signals unavailable to feature-based classifiers, and when combined with cryptographic integrity mechanisms they support architectures capable of detecting and attesting to anomalous behaviour.

6. Emerging Trends and Future Directions

Large-scale quantum computation poses a direct threat to the number-theoretic assumptions underlying widely deployed public-key cryptography, and NIST's post-quantum standardisation process has accelerated interest in graph- and lattice-based alternatives believed to resist known quantum algorithms (National Institute of Standards and Technology, 2020). Isogeny-based schemes such as CSIDH, which operate over Cayley-graph-like structures of isogenous elliptic curves, exemplify this trend and continue to be refined in response to ongoing cryptanalysis (Castryck *et al.,* 2018). Graph neural networks represent a second frontier, offering AI-assisted cryptanalysis and defence in which learned graph representations search for structural weaknesses in candidate constructions and strengthen intrusion-detection pipelines protecting cryptographic infrastructure (Wu *et al.,* 2021; Lo *et al.,* 2022).

A further direction concerns dynamic graph encryption, in which the underlying graph evolves in response to topology changes, device churn, or adversarial behaviour, requiring schemes that maintain security under continuous structural modification rather than a static graph — particularly relevant to IoT and sensor deployments with non-stationary connectivity. Promising research opportunities include systematic cryptanalysis of newly proposed graph families to establish concrete security margins, standardised benchmarks for graph-based post-quantum

candidates, tighter integration of graph neural networks into protocol design itself, and hybrid schemes combining graph-theoretic and lattice-theoretic assumptions to diversify risk in next-generation cryptographic infrastructure.

Conclusion

This chapter has traced the convergence of graph theory and cryptography from foundational concepts through concrete constructions and applied deployments across healthcare, the Internet of Things, blockchain, cloud computing, wireless sensor networks, artificial intelligence, and cybersecurity. The evidence surveyed demonstrates that graph-theoretic structures, particularly expander graphs, Cayley graphs, and spectral invariants, are not merely descriptive analogies for cryptographic systems but active generators of security guarantees, complementing and, in the post-quantum setting, increasingly supplementing classical number-theoretic foundations. At the same time, the cryptanalytic history of graph-based hash functions shows that expansion alone does not guarantee security, and continued mathematical scrutiny remains essential. As graph neural networks, dynamic network environments, and post-quantum standardisation mature, the integration of graph theory and cryptography is positioned to remain a central axis of discovery and application in information security research, embodying the bridging of fundamental science and practical technology that motivates this volume.

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QUATERNARY CHALCOGENIDES AND THEIR APPLICATIONS

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Introduction

Quaternary chalcogenides are complex solid-state materials containing four different elements, where at least one is a chalcogen (sulfur, selenium, or tellurium) combined with metal or semi-metal cations. They function as direct bandgap semiconductors with tunable optoelectronic properties, low thermal conductivity, and high structural stability [1]. Quaternary chalcogenides have recently been proposed as alternative absorbers. Their crystal structures and electronic properties are very similar to those of the parent CIGS, while their constituent elements are naturally abundant and nontoxic.

The I_2-II-IV-VI_4 quaternary chalcogenide semiconductors e.g. Cu_2ZnGeS_4, Cu_2ZnSnS_4, $Cu_2ZnGeSe_4$, $Cu_2CdSnSe_4$ and $Ag_2CdGeSe_4$ have been studied for more than 40 years but the nature of their crystal structures has proved contentious. Literature reports exist for the stannite and kesterite mineral structures, which are zinc-blende-derived structures. The I_2-II-IV-VI_4 (I=Cu,Ag; II=Zn,Cd; IV=Si,Ge,Sn; VI=S,Se) series of quaternary chalcogenide semiconductors have drawn wide interest for their potential application as solar-cell absorbers, photocatalysts for solar water splitting, thermoelectric materials, The wide application of these quaternary compounds comes from their increased chemical and structural freedom, which makes their physical properties more flexible relative to binary and ternary compounds [2].

Structure

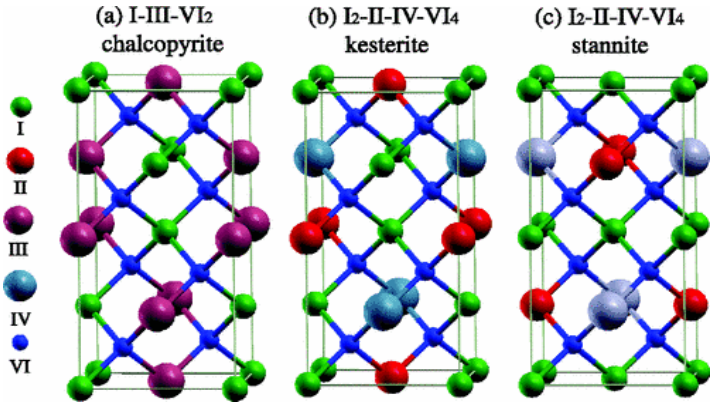

Figure 1: Structure of kesterite and stannite quaternary chalcopyrite and occupational differences of I and II group shown clearly

$Cu_2ZnSnSe_4$ (CZTSe) and $Ag_2ZnSnSe_4$ (AZTSe) (I_2 -II-IV-VI_4) are found to exit in Kesterite ($I\bar{4}$) structure but stannite ($I\bar{4}2m$) structure is also reported to exit due to occupational disorder of cations of I and II group [3]. Both the structure are Zinc Blende derived structures.

Kesterite structure and stannite structure differ only due to occupational disorder of cations of I and II group. Kesterite structure is found out to be the most stable structure in $Ag_2ZnSnSe_4$. Band gap of Kesterite $Ag_2ZnSnSe_4$ (0.94 eV) is wider than that of Kesterite $Cu_2ZnSnSe_4$ (0.63 eV) [4].

Applications

The I_2-II-IV-VI_4 (I= Cu,Ag; II= Zn,Cd; IV= Sn,Si; VI=Se,S) series of quaternary chalcogenide semiconductors have drawn wide interest for their potential application as

- Solar cell absorbers,
- Photocatalysis for solar water splitting,
- Thermoelectric materials.

The wide application of these quaternary compounds comes from their increased chemical and structural freedom, which makes their physical properties more flexible relative to binary and ternary compounds

Solar Cell Absorber

Solar energy in one form or another is the source of nearly all energy on the earth. Humans, like all other animals and plants, rely on the sun for warmth and food. However, people also harness the sun's energy in many other different ways. Photovoltaic (PV) is a simple and elegant method of harnessing the sun's energy. PV devices (solar cells) are unique in that they directly convert the incident solar radiation into electricity, with no noise, pollution or moving parts, making them robust, reliable and long lasting. Photons incident on the surface of a semiconductor will be either reflected from the top surface, will be absorbed in the material or, failing either of the above two processes, will be transmitted through the material. For photovoltaic devices, reflection and transmission are typically considered loss mechanisms as photons which are not absorbed do not generate power. If the photon is absorbed it has the possibility of exciting an electron from the valence band to the conduction band. A key factor in determining if a photon is absorbed or transmitted is the energy of the photon. Therefore, only if the photon has enough energy will the electron be excited into the conduction band from the valence band. Photons falling onto a semiconductor material can be divided into three groups based on their energy compared to that of the semiconductor band gap:

- ($E_{ph} < E_G$): Photons with energy E_{ph} less than the band gap energy E_G interact only weakly with the semiconductor, passing through it as if it were transparent.
- ($E_{ph} = E_G$): Photons with energy equal to the E_G have just enough energy to create an electron hole pair and are efficiently absorbed.
- ($E_{ph} > E_G$): Photons with energy much greater than the band gap are strongly absorbed. However, for photovoltaic applications, the photon energy greater than the band gap is wasted as electrons quickly thermalize back down to the conduction band edges.

The absorption coefficient determines how far into a material light of a particular wavelength can penetrate before it is absorbed. In a material with a low absorption coefficient, light is only

poorly absorbed, and if the material is thin enough, it will appear transparent to that wavelength. The absorption coefficient depends on the material and also on the wavelength of light which is being absorbed.

Characteristic properties of a photovoltaic material

- Absorption co-efficient should be high $>10^4$/cm.
- Proper band gap in the range of solar spectra which range from 1-5 eV. But we usually prefer to use material with the band gap in range of 1-1.5 eV to increase the efficiency of the device.
- Limited literature available on AZTSe show that band gap ~ 1.34 eV for film and ~ 0.94 eV for compound which makes it suitable for photovoltaic application [4].
- Hence an effort is put forth to understand structural, optical properties of it to utilize it as a photovoltaic material.

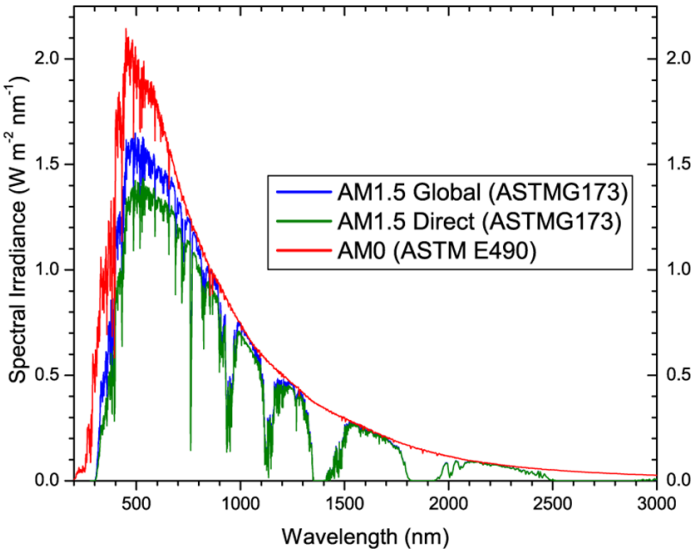

Figure 2: Solar Spectra

Photocatalytic Water Splitting

Photocatalytic water splitting is an artificial photosynthesis process used for the dissociation of water into its constituent parts, hydrogen (H_2) and oxygen (O_2), using either artificial or natural light. Hydrogen fuel production has gained increased attention as oil and other nonrenewable fuels become increasingly depleted and expensive. Methods such as photocatalytic water splitting are being investigated to produce hydrogen fuel, which burns cleanly and can be used in a hydrogen fuel cell. Water splitting holds particular interest since it utilizes water, an inexpensive renewable resource [6]. Photocatalytic water splitting has the simplicity of using a powder in solution and sunlight to produce H_2 and O_2 from water and can provide a clean, renewable energy, without producing greenhouse gases or having many adverse effects on the atmosphere. The process of water-splitting is a highly endothermic process ($\Delta H > 0$). Water splitting occurs naturally in photosynthesis when photon energy is absorbed and converted into the chemical energy through a complex biological pathway. However, production

of hydrogen from water requires large amounts of input energy, making it incompatible with existing energy generation. For this reason, most commercially produced hydrogen gas is produced from natural gas.

There are several strict requirements for a photocatalyst to be useful for water splitting. The minimum potential difference (voltage) needed to split water is 1.23V at 0 pH. Since the minimum band gap for successful water splitting at pH=0 is 1.23 eV corresponding to light of 1008 nm, the electrochemical requirements can theoretically reach down into infrared light, albeit with negligible catalytic activity [6]. Theoretically, infrared light has enough energy to split water into hydrogen and oxygen; however, this reaction is kinetically very slow because the wavelength is greater than 380 nm. The potential must be less than 3.0V to make efficient use of the energy present across the full spectrum of sunlight. Multinary semiconductor materials fulfill the band requirements outlined above and can be used in photocatalytic water splitting.

Thermoelectric Materials

Thermoelectric materials show the thermoelectric effect in a strong or convenient form. The thermoelectric effect refers to phenomena by which either a temperature difference creates an electric potential or an electric potential creates a temperature difference [7]. These phenomena are known more specifically as the Seebeck effect (converting temperature to current), Peltier effect (converting current to temperature), and Thomson effect (conductor heating/cooling). While all materials have a nonzero thermoelectric effect, in most materials it is too small to be useful. However, low-cost materials that have a sufficiently strong thermoelectric effect (and other required properties) could be used in applications including power generation and refrigeration. Semiconductors are ideal thermoelectric devices because of their band structure and electronic properties at high temperatures.

Refrigeration (Thermoelectric Cooling)

Thermoelectric materials can be used as refrigerators, called "thermoelectric coolers", or "Peltier coolers" after the Peltier effect that controls their operation. As a refrigeration technology, Peltier cooling is far less common than vapor-compression refrigeration. The main advantages of a Peltier cooler (compared to a vapor-compression refrigerator) are its lack of moving parts or circulating fluid, and its small size and flexible shape (form factor). Another advantage is that Peltier coolers do not require refrigerant fluids, such as chlorofluorocarbons (CFCs) and related chemicals, which can have harmful environmental effects [8]. The main disadvantage of Peltier coolers is that they cannot simultaneously have low cost and high-power efficiency. Advances in thermoelectric materials (new semiconductors) may allow the creation of Peltier coolers that are both cheap and efficient.

Power Generation (Thermoelectric Generators)

Approximately 90% of the world’s electricity is generated by heat energy, typically operating at 30–40% efficiency, losing roughly 15 terawatts of power in the form of heat to the environment.

Thermoelectric devices could convert some of this waste heat into useful electricity. Cogeneration power plants use the heat produced during electricity generation for alternative purposes. Thermoelectric may find applications in such systems or in solar thermal energy generation [9].

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WHOLE-GRAIN FOODS IN CARDIOVASCULAR HEALTH: BIOACTIVE COMPONENTS AND PROTECTIVE MECHANISMS

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Abstract

Cardiovascular disease remains a leading cause of premature mortality, emphasising the need for sustainable dietary strategies that modify multiple cardiometabolic risk factors. Whole-grain foods retain the bran, germ and endosperm, preserving a complex matrix of dietary fibre, resistant starch, phenolic compounds, phytosterols, vitamins and minerals that is substantially diminished during refining. This chapter examines the principal bioactive components of whole grains and their protective cardiovascular mechanisms. Soluble fibres, particularly oat and barley β-glucan, reduce low-density lipoprotein cholesterol by increasing intestinal viscosity, limiting bile-acid reabsorption and stimulating hepatic cholesterol utilisation. Fermentable fibres and resistant starch promote microbial production of short-chain fatty acids, potentially improving lipid metabolism, glucose regulation, vascular integrity and inflammatory balance. Phenolic acids, avenanthramides, tocopherols and alkylresorcinols provide complementary antioxidant and anti-inflammatory activities, while magnesium and potassium support vascular tone and blood-pressure regulation. Recent epidemiological evidence associates greater whole-grain intake with reduced risks of coronary heart disease, stroke, hypertension and cardiovascular mortality. However, responses vary according to grain species, food structure, processing intensity, bioactive concentration and individual metabolic characteristics. Intact or minimally processed oats, barley, rye, whole wheat, brown rice and millets may consequently provide stronger benefits than finely milled or highly sweetened products carrying whole-grain claims. Whole grains should replace refined cereals within balanced dietary patterns rather than be consumed as isolated additions. Preserving the complete grain matrix offers a practical, culturally adaptable and sustainable pathway for improving cardiovascular health.

Keywords: Whole Grains, Cardiovascular Disease, B-Glucan, Dietary Fibre, Phenolic Compounds, Cardioprotection.

1. Introduction

Cardiovascular disease encompasses coronary heart disease, stroke, heart failure and related vascular disorders driven by dyslipidaemia, hypertension, insulin resistance, oxidative stress and chronic inflammation. Dietary modification remains fundamental to prevention because it can

simultaneously influence these interconnected pathways. Whole grains are particularly valuable because they retain the bran, germ and endosperm, delivering fibre, micronutrients and phytochemicals within a naturally organised food matrix.

Their cardiovascular effects extend beyond the conventional contribution of dietary fibre. β-Glucan, resistant starch, arabinoxylans, phenolic acids, phytosterols, tocopherols, alkylresorcinols and minerals may collectively regulate cholesterol metabolism, endothelial function, inflammatory signalling and microbial activity. Nevertheless, whole-grain products are not physiologically equivalent. Grain species, particle size, milling, extrusion, fermentation, cooking and added ingredients can substantially alter nutrient accessibility and metabolic response. This chapter evaluates the major cardioprotective constituents of whole grains, their underlying biological mechanisms, the strength of recent evidence and the priorities required to translate whole-grain science into effective cardiovascular nutrition.

2. Bioactive Architecture of Whole Grain

A whole-grain kernel contains the fibre-rich bran, lipid- and micronutrient-rich germ and starch-dominant endosperm. Maintaining these fractions preserves an integrated combination of fermentable and non-fermentable fibres, vitamins, minerals and phytochemicals. Oats and barley are distinguished by soluble β-glucan, whereas wheat and rye contribute arabinoxylans, cellulose, lignin and substantial insoluble fibre. Brown rice, sorghum and millets provide varying concentrations of resistant starch, phenolic compounds and minerals (Guo *et al.,* 2022).

Phenolic acids—including ferulic, caffeic, p-coumaric, sinapic and vanillic acids—are concentrated in the outer kernel layers. Their antioxidant and signalling activities may restrict lipid oxidation, inflammatory activation and endothelial injury. Oats additionally contain avenanthramides, which possess antioxidant and anti-inflammatory properties and may enhance nitric-oxide-mediated vascular function. Tocopherols, tocotrienols, phytosterols, carotenoids and alkylresorcinols provide further biological functionality (Valladares *et al.,* 2024).

The health effect arises from interactions among these constituents rather than from a single compound. Removal of the bran and germ therefore eliminates not only fibre but also a coordinated bioactive network. Conversely, excessive milling may disrupt cellular architecture and accelerate nutrient digestion even when all anatomical fractions remain present. Whole-grain functionality consequently depends on both composition and structural integrity.

3. Cholesterol and Bile Acid Metabolism

The lipid-lowering action of cereal β-glucan is among the strongest established mechanisms supporting cardiovascular protection. Following hydration, high-molecular-weight β-glucan increases intestinal viscosity and restricts bile-acid reabsorption. Greater faecal bile-acid excretion stimulates hepatic conversion of cholesterol into new bile acids and can enhance LDL-receptor-mediated clearance of circulating cholesterol.

Meta-analytic evidence demonstrates that oat β-glucan lowers total and LDL cholesterol, with stronger effects observed among individuals with hyperlipidaemia and after longer interventions (Yu *et al.,* 2022). Both whole-oat foods and isolated β-glucan preparations improve lipid profiles, although the complete grain may provide broader effects through its phenolic compounds, minerals and complementary fibres (de Morais Junior *et al.,* 2023). Barley β-glucan operates through similar viscosity-dependent and bile-acid-mediated pathways.

Physiological efficacy is influenced by β-glucan dose, solubility and molecular weight. Aggressive processing can depolymerise β-glucan, decrease viscosity and weaken cholesterol reduction. Thus, two products containing identical amounts of β-glucan may not generate equivalent outcomes. Recent reviews recommend assessing physicochemical functionality alongside declared fibre content when evaluating cardiovascular benefits (McCarthy *et al.,* 2025).

Whole grains also provide phytosterols that compete with cholesterol for intestinal absorption. Fermentation of cereal fibres produces short-chain fatty acids, particularly propionate, which may influence hepatic lipid synthesis. These pathways collectively support reductions in atherogenic lipoproteins rather than merely changing total cholesterol.

4. Vascular and Blood Pressure Regulation

Endothelial dysfunction is an early event in atherosclerosis and is characterised by impaired nitric oxide activity, oxidative stress and abnormal vascular reactivity. Whole-grain phenolics may protect nitric oxide from oxidative degradation and regulate signalling pathways involved in vasodilation. Avenanthramides may further suppress vascular inflammation and support endothelial nitric oxide production.

Whole grains supply magnesium and potassium, minerals involved in vascular smooth-muscle relaxation, electrolyte balance and blood-pressure control. Dietary fibre may additionally support weight management and insulin sensitivity, indirectly reducing haemodynamic stress. A systematic review found that oat consumption produced a modest but significant reduction in systolic blood pressure, although responses varied with participants' baseline health and intervention characteristics (Xi *et al.,* 2023).

Recent dose–response evidence also associates higher whole-grain consumption with a lower incidence of hypertension. Benefits appear particularly meaningful when whole grains replace refined carbohydrates rather than simply increasing total energy intake (Aune *et al.,* 2025). Reduced postprandial glycaemia and insulinaemia may further protect vascular function by limiting oxidative stress, arterial stiffness and glycation-related endothelial injury (Li *et al.,* 2023).

5. Gut Microbiota, Oxidative Stress and Inflammation

Fermentable cereal fibres and resistant starch reach the colon, where they are metabolised by intestinal microorganisms. This process produces acetate, propionate and butyrate, which support epithelial-barrier integrity and interact with receptors involved in immune regulation, lipid metabolism and vascular tone. Whole-grain cereals may also increase microbial diversity and promote beneficial bacterial groups, although responses depend on grain type, fibre structure and the host microbiome (Comerford, 2026).

Strengthening the intestinal barrier may reduce systemic exposure to pro-inflammatory microbial products. This is relevant because persistent low-grade inflammation contributes to endothelial dysfunction, plaque development and metabolic dysregulation. Phenolic metabolites generated during colonic fermentation may provide additional systemic antioxidant and anti-inflammatory activity.

Whole-grain dietary patterns may influence inflammasome-mediated signalling. Balanced diets rich in fibre and plant-derived antioxidants can potentially suppress excessive activation of the NLRP3 inflammasome, which is implicated in metabolic inflammation and vascular injury (van der Heiden & te Velde, 2026). The observed cardiovascular effect is therefore likely to reflect communication among the grain matrix, intestinal microbiota, immune system, liver and vascular endothelium.

6. Cardiovascular Evidence and Dietary Application

Prospective studies consistently associate higher whole-grain intake with lower cardiovascular incidence and mortality. A recent systematic review found that whole-grain consumption, compared with refined-grain intake, was associated with reduced coronary heart disease, cardiovascular events and all-cause mortality (Hu *et al.,* 2023). Dose–response analyses further support replacing refined cereals with whole grains as the principal dietary grain source (Liu *et al.,* 2024).

Controlled trials generally demonstrate modest improvements in LDL cholesterol, blood pressure, postprandial metabolism and inflammatory markers. Oat-based interventions provide particularly consistent lipid-lowering evidence, whereas findings for other grains remain heterogeneous (Llanaj *et al.,* 2022; Mathews *et al.,* 2025). The difference partly reflects variation in intervention duration, processing, grain dose, comparator foods and participant risk profiles.

Clinical application should prioritise substitution and variety. Steel-cut or rolled oats, barley, rye, whole-wheat kernels, brown rice and minimally processed millets can replace refined bread, polished rice and low-fibre cereals. Whole grains are most protective within diverse dietary patterns containing vegetables, fruits, pulses, nuts and unsaturated fats (Ridwan *et al.,* 2026). Added sugars, sodium and saturated fats must also be considered because they can diminish the cardiovascular value of commercial whole-grain products.

7. Challenges and Future Perspectives

Whole-grain research must progress from compositional labels towards **functional precision**. Products containing identical whole-grain percentages can differ substantially in kernel integrity, particle size, β-glucan molecular weight, added sugars and metabolic effects. Existing studies also vary in serving definitions, grain species, comparators, duration and cardiovascular endpoints, limiting evidence synthesis (Hu *et al.,* 2023).

Future trials should characterise foods by processing severity, starch accessibility, fibre functionality and phytochemical bioavailability. Longer multicentre interventions should incorporate apolipoprotein B, continuous glucose monitoring, ambulatory blood pressure, endothelial function, inflammatory mediators, microbiome profiles and cardiovascular events. Biomarkers such as alkylresorcinols could objectively confirm adherence.

The brightest opportunity is precision whole-grain nutrition: matching oats, barley, rye, wheat, brown rice or millets to individual lipid, glycaemic and microbial phenotypes. Fermentation, germination and controlled thermal processing could improve bioactive accessibility while preserving structural resistance to digestion (Valladares *et al.,* 2024). Affordable, culturally familiar convenience foods must also be developed. Tomorrow's whole-grain product should not merely contain the complete kernel; it should retain measurable functionality and demonstrate a clinically meaningful cardiovascular advantage.

Conclusion

Whole-grain foods offer a biologically plausible and nutritionally comprehensive strategy for cardiovascular protection. Their retained bran, germ and endosperm provide dietary fibre, resistant starch, phenolic acids, phytosterols, avenanthramides, tocopherols, alkylresorcinols and essential minerals within an interactive food matrix. These constituents influence several interconnected determinants of cardiovascular disease, including atherogenic cholesterol, bile-acid metabolism, blood pressure, postprandial glucose regulation, oxidative stress, inflammation, endothelial function and intestinal microbial activity.

The cholesterol-lowering effect of viscous oat and barley β-glucan represents the most firmly established mechanism. Nevertheless, the value of whole grains cannot be reduced to a single fibre fraction. Phenolic compounds support antioxidant and inflammatory regulation, minerals contribute to vascular homeostasis, and fermentable carbohydrates generate microbial metabolites capable of influencing systemic metabolism. Preservation of physical structure is equally important because extensive milling, extrusion and formulation with added sugars may diminish metabolic benefits despite the retention of whole-grain ingredients.

Recent observational evidence consistently associates greater whole-grain intake with lower cardiovascular risk and mortality. Intervention studies provide more direct support for improvements in intermediate risk markers, particularly lipid profiles and blood pressure,

although long-term clinical-event evidence remains limited. Whole-grain foods should consequently complement rather than replace established cardiovascular treatments and lifestyle interventions.

Their greatest protective potential emerges when intact or minimally processed grains replace refined cereals within dietary patterns rich in vegetables, fruits, pulses, nuts and unsaturated fats. Product choice must consider grain type, processing, fibre functionality, added ingredients and individual metabolic tolerance. A grain becomes genuinely heart-protective when its structure remains intact, its bioactive matrix remains functional and it replaces—not accompanies—a refined carbohydrate.

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HIERARCHICALLY POROUS CARBON FROM LEAF BIOMASS FOR SUPERCAPACITOR AND BATTERY APPLICATIONS

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Abstract

The increasing global demand for clean and sustainable energy, together with the depletion of fossil fuel resources and growing environmental concerns, has accelerated the development of advanced energy storage technologies. Among various electrode materials, biomass-derived porous carbon has attracted significant attention owing to its renewability, low cost, high specific surface area, excellent electrical conductivity, and outstanding thermal and chemical stability. In particular, leaf biomass is an abundant and sustainable carbon precursor for producing hierarchically porous carbon with interconnected pore networks that promote rapid ion transport and enhanced electrochemical performance. This chapter reviews recent advances in the synthesis, activation strategies, structural characteristics, and electrochemical properties of leaf-derived hierarchically porous carbon for energy storage applications. Particular emphasis is placed on its use as an electrode material in supercapacitors and rechargeable batteries, where its unique pore architecture improves electrolyte accessibility, charge storage capacity, rate capability, and cycling stability. The effects of pore structure, surface functional groups, and activation methods on electrochemical performance are also discussed. Finally, the chapter highlights the environmental and economic benefits, current challenges, and future prospects of leaf derived porous carbon, demonstrating its strong potential as a sustainable electrode material for next generation high-performance electrochemical energy storage systems.

1. Introduction

In the rushed development of human life, a huge amount of power expenditure and energy has been utilized by human beings for different types of applications, such as civilization and industrilization. Besides, the increasing energy requirement and environmental pollution in current society, though avoiding resource consumption and the world while pollution protection is the most important task to our human society, require innovative, with high performance, non-pollutant and low cost energy storage and conversion systems. Nowadays, energy plays a more important role in economic and industrial development. The major expenditure of non-renewable energy sources is the utilization of fossil fuels, including oil, coal and natural gas, considerably due to the global economic and population detonation. And also, the universal energy and

chemical producers of non-renewable resources such as oil and natural gas may cease the excessive use of these this resources after 40 years [1].

However, the energy derived from different types of power production resources available, is non-renewable, with a minimum stage of remaining source. Moreover, the excess use of fossil fuel resources will surely vanished in the coming years, which means that excess use of resource will meet some more problems in the future like the major issue of environmental pollution which is rising day by day. Also, the uncontrolled exploitation of natural resource and fossil fuel is more than 10.000 times higher than with the production of fossil fuels through natural sources. With that different type of gas created in the environment, greenhouse gas emissions (such as: CO_2, CH_4, NO_2, SO_2 and fly ash) result from the utilization of fossil fuels, which are owing to cause severe environmental pollution and global worming (the greenhouse effect) [2-4]. From this problem, there is an imperative requirement to create more suitable power producing technology and energy storage devices before the destruction of natural resources.

Further, the high deployment of fossil fuels causes greenhouse gases and has emerged as an environmental problem with limited supply in the world. Renewable energy is more suitable for sustainable as well as sanitary and environmentally friendly materials. In response to the above issues, the desire for the development of high efficient, low cost, non-pollut in green, renewable energy storage and production technology is well in demand in the current world. Recently, most of the researchers focused on the perfection of high performance of energy storage devices like fuel cells, supercapacitor batteries (particularly: Li-ion battery) and solar cells and so on. These are some of the most capable alternative processes. However, we utilized the advanced key feature to solve the problem of fundamentals with enhanced material development for energy conversion and storage processes. The good performance material has specific structure, characterization and definite properties its naturally designed for innovative application as well as good energy storage and conversion in the chemical fields. And also, it conserves the environment and the cost effective production of these materials is relatively simple and green, renewable abundant.

However, energy can be derived from other way of the renewable resources such as wind, solar, tidal, natural gas and other natural resources and also, the energy production of this method is superb compared to other production routes. Thus, there is a need for more capable energy storage techniques for alteringenergy from one form to another with long durability. Moreover, a good energy storage technique requires saving energy losses with in a cost effective manner. Nowadays, there are different types of energy conversion and storage techniques available like batteries, supercapacitor, electrochemical device, solar cell, conversional capacitor and fuel cell. Among the energy conversion and storage devicessupercapacitor and electrochemical capacitors

are more accessible due to their amazing properties of long cycle life, good charge/discharge capability, non-pollution, high energy density and excellent operation safety [5-7].

2. Porous Carbon Prepared from Leaf Biomass

In leaves based porous carbon has great attention in the research fields, which is renewable and low cost carbon material. Some leaves based carbon works Rawal *et al.* [8] reported the saccharum bengalense derived activated carbon (SbAC) for supercapacitor through simple carbonization approach. The SbAC electrode achieved a high specific capacitance of 102.6 F g^{-1} at 2 mVs^{-1} and found good cyclic strength after 120,000 cycles in 1M Li_2SO_4 electrolyte. From the results clearly indicate that SbAC can be a better electrode material for supercapacitor. Yan *et al.* [9] fabricated the hierarchically porous activated carbons (HPACs) through pre-carbonization method by utilizing Schefflera octophylla leaves as a carbon precursor. They found that HPACs electrode delivered a superb electrochemical performance with specific capacitances of 336 F g^{-1} at 0.5 A g^{-1}, 220 F g^{-1} at 5 A g^{-1} and 200 F g^{-1} at 10 A g^{-1} respectively and also, showed an excellent cyclic capability of 97.5 % initial capacitance over 10000 cycles in 6 M KOH electrolyte at 10 A g^{-1}. Moreover, the as-assembled HPACs electrode based symmetric supercapacitoe device achieved the amazing energy density of 47.5 Wh kg^{-1} and at 71.9 W kg^{-1} and retained the best energy density of 22.1 Wh kg^{-1} and maximum energy density of 47.5 Wh kg^{-1} using 6 M KOH electrolyte. He *et al.* [10] reported the nitrogen, sulfur dual-doped ladder like porous carbon (NSLPC) for suppercapacitor through a simple carbonization route from mulberry leaves as a carbon precursor. The NSLPC based electrode achieved a very high super specific capacitance of 214.5 F g^{-1} at 0.5 A g^{-1} compare to NLPC (185.5 F g^{-1} at 0.5 Ag^{-1}) and LPC (165 F g^{-1} at 0.5 A g^{-1}) with delivered the excellent cyclic life strength of 94 % initial capacitance hold over 5000 cycles at 3 A g^{-1} and expended 90.2% initial specific capacitance maintain 20000 s under 6 M KOH solution. Zhu *et al.* [11] fabricated the dead ginkgo leave derived porous carbon (KGC) for supercapacitor via simple carbonization method. The observed KGC electrode has a very high specific capacitance of 374 F g^{-1} at 0.5 A g^{-1} using 1 M H_2SO_4 electrolyte and also possessed the remarkable life cycle strength of 77 % initial capacitance maintain over 2000 cycles and expended 71 % capacitance keep over 5000 cycles at 4 A g^{-1} under 1 M H_2SO_4 electrolyte. Also, the fabricated KGC electrode based symmetric supercapacitor device exhibited super specific capacitance of 272 F g^{-1} at 0.2 A g^{-1} with achieved an excellent power density of 48 W kg^{-1} and energy densities of 2-5 Wh kg^{-1}. Sankar *et al.* [12] utilized the green-tea wastes to derive the TWA-WC for supercapacitor from simple and low-cost carbonization method. The TWA-WC electrode showed an amazing specific capacitance of 162 F g^{-1} at current density of 0.5 A g^{-1} in 1 M H_2SO_4 electrolyte. In addition, the TWA-WC electrode delivered very high capacitance of 121 % retention over 5000 cycles at 0.5 Ag^{-1}. The

FE-SEM images of (a) TWA as a raw source material, (b) KOH-activated TWA, (c) TWA-HC nanoparticles, and (d) TWA-WC nanoflakes are shown in Fig.6.

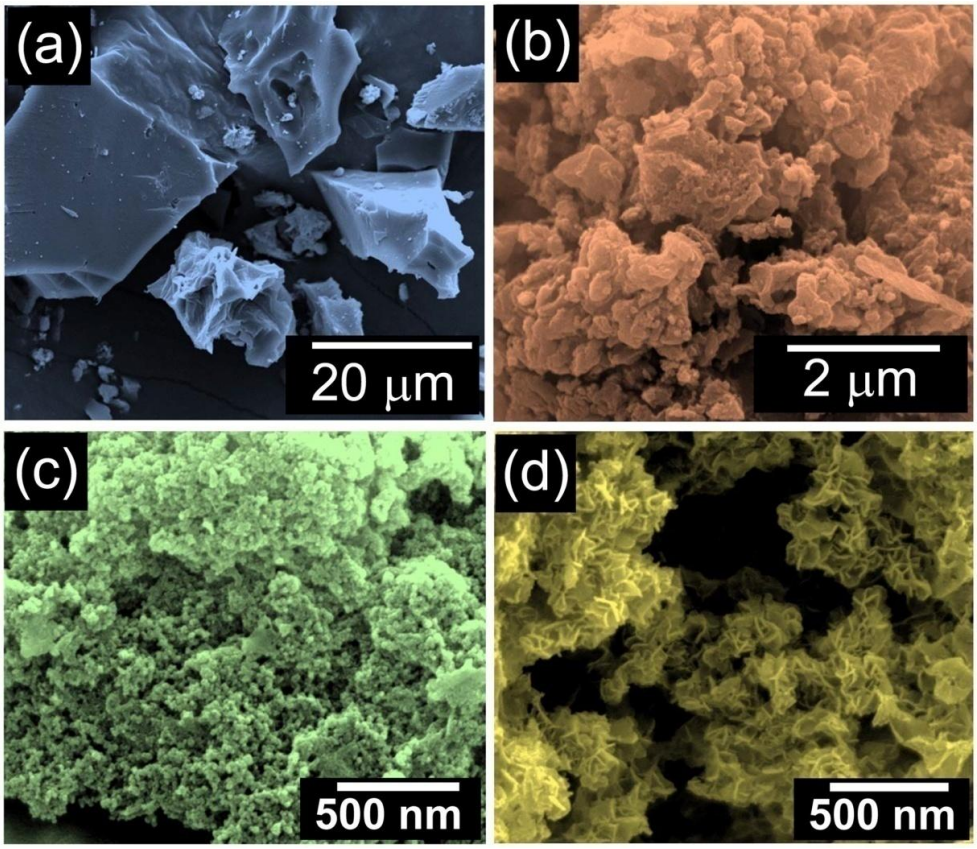

Figure 1: FE-SEM images of (a) TWA as a raw source material, (b) KOH-activated TWA, (c) TWA-HC nanoparticles, and (d) TWA-WC nanoflakes [12], (Copyright 2019, Elsevier)

Zhang *et al.* [13] fabricated the 3D hierarchical petal-like $Co_xNi_{3-x}Si_2O_5(OH)_4/C$ composites derived by bamboo leaves using combined method of hydrothermal and carbonization process and also the obtained electrode material utilizing for supercapacitor application. The prepared $Co_xNi_{3-x}Si_2O_5(OH)_4/C$ composites showed a good electrode chemical performance with delivered an excellent specific capacitance of 226 F g^{-1} in 3 M KOH as an electrolyte at 0.5A g^{-1} with exhibited the significant cyclic durability of 99 % capacitance keep over 10000 cycles at 15 A g^{-1}. Besides, the as-assembled CoNiSi/C//$Ni(OH)_2$ electrode based device achieved excellent capacitance of 64 F g^{-1} with showed a very good energy density of 20.0 Wh kg^{-1} and power density of 94.5 W kg^{-1} and also produced best life cycle stability of 82 % initial specific capacitance maintain over 10000 cycles at 1 A g^{-1}. In Fig.7 shows the schematic illustration for synthetic strategy of 3D CoNiSi/C with layered structure of CoNiSi.

Yu *et al.* [14] synthesized the porous carbons for supercapacitor through carbonization technique from the onion leaves as a carbon resource. The offered electrode showed the good electrochemical performance with achieved remarkable specific capacitance of 158.6 F g^{-1} at 0.2 A g^{-1} in 3 M KOH electrolyte with showed the better cyclic only 4 % rate decay over 5000

cycles at 10 A g^{-1}. From the result suggested that the obtained electrode material suitable for supercapacitor application.

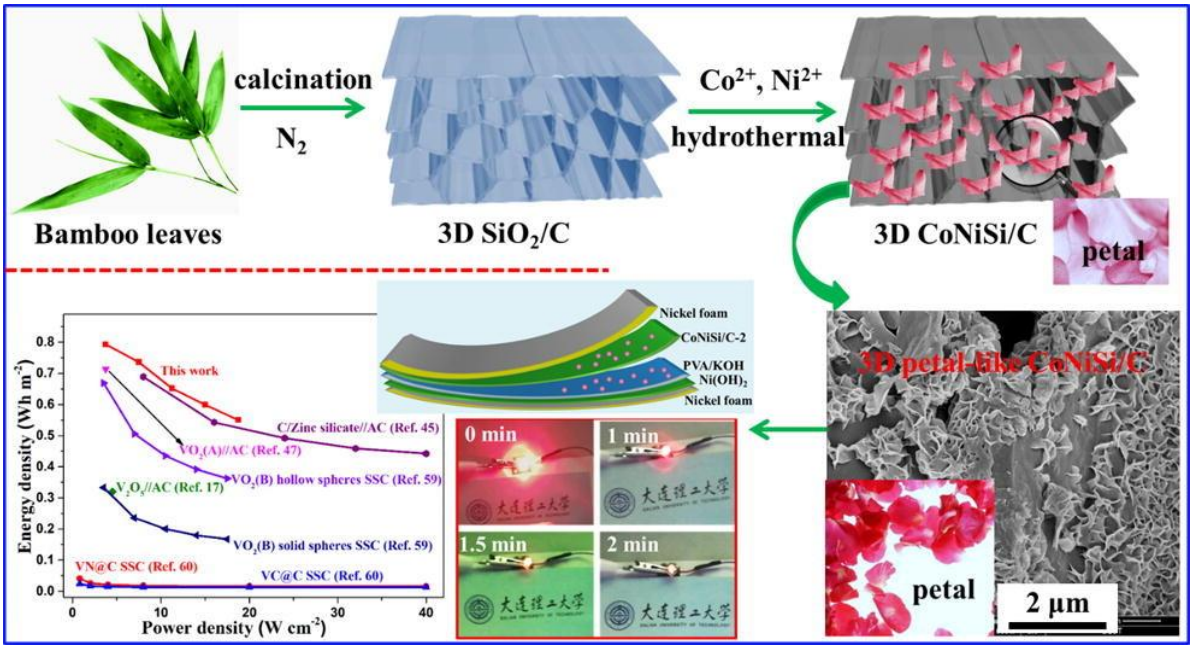

Figure 2: The schematic illustration for synthetic strategy of 3D CoNiSi/C with layered structure of CoNiSi [13] (Copyright 2019, Elsevier)

Song *et al.* [15] developed the activate carbon (TC1200) derived from tea waste as a resource through pre-carbonization method. They noted that obtained electrode material has a high specific capacitance of 167 F g^{-1} at current density of 1 A g^{-1} with exhibited a very good electrochemical performance of life cycle stability of 96.66% keep over 16000 cycles at 4 A g^{-1} using 6 M KOH electrolyte. Moreover, the fabricated TC1200 based symmetric supercapacitor device has an excellent energy density of 33,494.70 W kg^{-1} and power density of 19.45 Wh kg^{-1} in 1 M Na_2SO_4 electrolyte at 4 A g^{-1}. Jin *et al.* [16] utilized the rice straw to derive 3D interconnected porous graphitic carbon (3D-IPGCs) for supercapacitor from carbonization method. The 3D-IPGCs based electrode offered a good electrochemical performance with excellent specific capacitance of (400 F g^{-1}), (312 F g^{-1}) and (232.2 F g^{-1}) at 0.1 A g^{-1}, 5 A g^{-1} and 5 A g^{-1} respectively and also has a best cyclic performance of only loss 6.4% initial specific capacitance over 10000 cycles in 6 M KOH as an electrolyte at current density of 5 A g^{-1}. Besides, the as-assembled 3D-IPGCs electrode based symmetric device produce has very good power density from 13.9 Wh kg^{-1} at 0.025 kW kg^{-1} to 10.8 Wh kg^{-1}at 1.258 kW kg^{-1} and expended energy density 8.06 Wh kg^{-1}at 12.85 kW kg^{-1}. Qu *et al.* [17] reported the lotus leaf derived porous carbon (LLPC) through a simple carbonization approach for supercapacitor. The obtained LLPC suggested that the good specific capacitance of 379 F g^{-1} at 1 A g^{-1} with exposed has a superior life specific capacitance of 298 F g^{-1} and achieved excellent cyclic stability of 90% keep over 5000 cycles at current density of 20 A g^{-1} using 6 M KOH electrolyte. Moreover, the

prepared LLPC-800-1:3//LLPC-800-1:3 electrodes based symmetric device reached the energy density of 9.2 Wh kg^{-1} and power density of 491W kg^{-1} under 1 M Na_2SO_4 electrolyte.

Table 1: Electrochemical performances of leaves biomass based porous carbon for supercapacitor applications

Porous Carbon Resource	Method	Capacitance ($F\ g^{-1}$)	Current Density ($A\ g^{-1}$)	Electrolytes	Ref.
Saccharum bengalense	Hydro	102.6	$2mVs^{-1}$	1M Li_2SO_4	8
Schefflera octophylla	Hydro	336	0.5	6 M KOH	9
Mulberry leaves	Hydro	214.5	0.5	6 M KOH	10
Ginkgo leave a	Hydro	374F	0.5	1 M H_2SO_4	11
green-tea wastes	Hydro	162	0.5	1 M H2SO4	12
Bamboo leaves	Hydro	226	0.5	3 M KOH	13
Onion leaves	Hydro	158.6	1	3 M KOH	14
Tea waste	Hydro	167	1	6 M KOH	15
Rice straw	Hydro	400	0.1	6 M KOH	16
Lotus leaf	Hydro	379	1	6 M KOH	17

Conclusion

Leaf based porous carbon has emerged as a highly promising and sustainable electrode material for high-performance supercapacitors owing to its renewable nature, low cost, environmental friendliness and naturally porous structure. The studies reviewed demonstrate that various biomass sources including Saccharum bengalense, Schefflera octophylla, mulberry leaves, dead ginkgo leaves and green tea waste can be successfully converted into porous carbon with excellent electrochemical properties through simple and cost effective carbonization and activation processes. These materials exhibit high specific capacitance, excellent rate capability, superior cycling stability and impressive energy and power densities, making them attractive candidates for nextgeneration energy storage devices. Furthermore, heteroatom doping and hierarchical pore engineering significantly enhance ion transport, electrical conductivity and charge storage performance. Although remarkable progress has been achieved, challenges such as scalable production, precise control of pore architecture, reproducibility and long term device stability still need to be addressed for commercial applications. Future research should focus on developing green and scalable synthesis strategies, optimizing heteroatom doping understanding the charge storage mechanisms and integrating leaf derived porous carbons into flexible and hybrid energy storage systems. Overall, leaf based porous carbons represent a sustainable and highly efficient class of electrode materials with significant potential for advancing environmentally friendly and cost effective supercapacitor technologies.

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NUTRIMIX FUSION: AN INNOVATIVE APPROACH TO ADDRESS MALNUTRITION AND NUTRITIONAL SECURITY

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1. Introduction

Malnutrition remains one of the most persistent and multidimensional public health challenges of our time, affecting populations across both developing and developed nations, with developing countries such as India bearing a disproportionate share of the burden (World Health Organization; Branca *et al.,* 2023). Malnutrition is not a single condition but a spectrum of nutrient intake imbalances — encompassing undernutrition (stunting, wasting, and underweight), micronutrient-related deficiencies, and overnutrition (overweight and obesity) — a coexistence often referred to as the "double burden of malnutrition" (Branca *et al.,* 2023).

A particularly insidious dimension of this problem is *hidden hunger*: a state in which individuals consume sufficient calories to avoid the visible signs of hunger, yet remain deficient in essential micronutrients such as iron, iodine, zinc, folate, and vitamins A, B12, C, and D (Food and Agriculture Organization; FAO Expert Panel, 2022). Because hidden hunger produces no immediately visible symptoms, it is frequently overlooked in public health planning, even though its long-term consequences — impaired cognitive development, weakened immunity, reduced productivity, and increased maternal and child mortality — are severe and often irreversible (UNICEF; Black *et al.,* 2023).

The scale of the problem is staggering. Global estimates indicate that more than two billion people worldwide are affected by chronic micronutrient deficiency, with recent analyses suggesting that over half of the world's population has an inadequate intake of at least one essential micronutrient (Micronutrient Forum, 2023; WorldHealth.net, 2026). Anaemia caused by iron deficiency alone affects an estimated 40 percent of children aged 6–59 months and nearly 30 percent of women of reproductive age globally, while iodine deficiency — the single leading preventable cause of intellectual disability worldwide — continues to place close to a third of the global population at risk (World Health Organization; Branca *et al.,* 2023). Roughly 334 million children and adolescents in low- and middle-income countries are estimated to be affected by vitamin A deficiency (WorldHealth.net, 2026).

India illustrates this challenge with particular urgency. Despite decades of agricultural growth and improvements in national food supply, the country continues to struggle to translate caloric sufficiency into nutritional adequacy for its population (IIPS & ICF, 2021). According to the

fifth National Family Health Survey (NFHS-5, 2019–21), 35.5 percent of Indian children under five are stunted, 19.3 percent are wasted, and 32.1 percent are underweight, while severe anaemia affects 57 percent of women of reproductive age (IIPS & ICF, 2021). More recent United Nations estimates place India's child wasting rate at 18.7 percent in 2024 — the highest of any country in the world — with over 21 million children affected, alongside roughly 37 million stunted children nationally (UN State of Food Security and Nutrition in the World [SOFI] Report, 2025). Anaemia among women has continued to rise rather than fall, from around 50 percent in 2012 to nearly 54 percent in 2023, representing over 200 million affected women (SOFI Report, 2025). These figures make clear that malnutrition in India is not a residual problem awaiting the natural effects of economic growth, but an active and, in some indicators, worsening crisis that demands targeted nutritional interventions.

It is within this context that the present chapter introduces and examines "Nutrimix Fusion," a proposed composite food product designed to deliver a balanced combination of macronutrients and micronutrients in a single, affordable, and culturally acceptable format.

2. Problem Statement

The persistence of malnutrition — and particularly of micronutrient deficiencies — despite decades of agricultural and food-industry development points to a fundamental inadequacy in how commercially available food products are formulated (Branca *et al.,* 2023). Most mass-market food products, including many marketed as "nutritious" or "fortified," are designed primarily to deliver calories and palatability rather than a comprehensive nutrient profile. Diets built around a narrow range of staple cereals — rice, wheat, or maize — tend to be energy-dense but micronutrient-poor, a pattern that has been described as a paradox of modern agricultural intensification: increased yields of high-yielding staple varieties have, in some respects, come at the cost of dietary diversity and micronutrient density (Yilmaz & Yilmaz, 2025).

This raises the central question addressed in this chapter: are currently available food products sufficient to meaningfully address malnutrition, particularly hidden hunger, in vulnerable populations? The evidence suggests they are not. Existing dietary interventions are frequently ineffective among low-income communities, whose limited purchasing power constrains access to diverse, nutritionally balanced diets (World Bank; Bredenkamp *et al.,* 2022). Even where fortified or supplementary foods exist, uptake is often limited by cost, poor sensory acceptability, and mismatches with local food cultures (FAO; Burlingame & Dernini, 2022). The result is a persistent gap between the theoretical availability of nutritious food and its actual, sustained consumption by the populations who need it most.

3. Need for the Product: Nutrimix Fusion

Addressing this gap requires food products that are simultaneously nutritious, affordable, and practical to produce and distribute at scale (FAO; Burlingame & Dernini, 2022). Nutrimix

Fusion is proposed as such a product: a composite food formulation engineered to combine macronutrients (proteins, carbohydrates, and healthy fats) with a targeted spread of essential micronutrients — including iron, zinc, iodine, folate, and vitamins A, B-complex, C, and D — within a single, easy-to-consume format.

The rationale for this approach is well supported in the nutrition literature. Composite and fortified foods are widely regarded as among the most cost-effective strategies for addressing micronutrient malnutrition at population scale, precisely because they integrate nutritional correction into foods that are already part of routine consumption, rather than requiring behavioural change alone (World Health Organization; Branca *et al.,* 2023; UNICEF; Black *et al.,* 2023). Multi-micronutrient fortification strategies — whether applied to staples such as wheat flour, salt, or sugar, or delivered through composite blended foods — have demonstrated measurable improvements in biochemical indicators such as haemoglobin, serum ferritin, and serum retinol levels, particularly among children and women of reproductive age (FAO, 2002; Fahmida *et al.,* Indonesia systematic review, 2021). Similarly, fortified blended foods and ready-to-use supplementary foods, long used in humanitarian and public nutrition programmes for children aged 6–59 months, have been progressively reformulated to improve both their nutrient density and their sensory acceptability (Research on fortified blended food aid products, 2024).

Nutrimix Fusion is designed to draw on these established principles while addressing two populations identified as being at the highest nutritional risk: children under five, for whom micronutrient deficiency during the critical window of growth can produce irreversible cognitive and physical impairment, and pregnant and lactating women, for whom deficiencies materially increase the risk of adverse birth outcomes and maternal morbidity (World Health Organization; Branca *et al.,* 2023).

4. Market Disadvantages and Existing Gaps

Despite the demonstrated effectiveness of fortification and composite-food strategies, several structural constraints limit the impact of currently available nutritional products.

- **Cost and urban bias:** A large proportion of fortified and nutrient-dense packaged foods are priced for, and marketed toward, urban and middle-income consumers, leaving rural and economically disadvantaged populations — who often carry the greatest nutritional burden — comparatively underserved (World Bank; Bredenkamp *et al.,* 2022).
- **Acceptability:** Even where affordable fortified products exist, low acceptance due to unfamiliar taste, texture, or preparation requirements can undermine sustained consumption. Products that do not align with local culinary traditions or ease of use are frequently abandoned after initial trial, regardless of their nutritional merit (FAO; Burlingame & Dernini, 2022).

- **Nutritional literacy:** A persistent and often underestimated barrier is the limited public understanding of what constitutes a balanced diet. Even where nutritious products are accessible and affordable, low awareness of micronutrient needs can suppress demand and reduce sustained uptake — an issue that nutrition education and product design must address jointly rather than in isolation.
- **Bioavailability and stability:** Technical constraints also persist. Certain micronutrients, particularly iron and vitamin A, are prone to degradation during storage or processing, and their bioavailability can be reduced by interactions with other food components, such as the phytates present in cereal-heavy diets (Discover Food, Springer Nature, 2025). Overcoming these constraints requires deliberate formulation choices — such as the use of chelated minerals, encapsulation techniques, or complementary ingredient pairing — to preserve nutrient potency from production through to consumption.

Taken together, these gaps indicate that an effective nutritional product must be engineered not only for nutrient content, but for cost, taste, cultural fit, and stability — the full set of factors that determine whether a nutritious product is actually and consistently consumed.

5. Need for Innovation in Food Product Development

Meeting these combined requirements calls for genuine innovation in food science and product design, rather than incremental adjustments to existing offerings (Food Technology; Fellows, 2017). One promising direction is the deliberate integration of indigenous and locally available foods — pulses, millets, oilseeds, and regional cereals — with modern food-processing techniques capable of preserving or enhancing nutrient content while extending shelf life (FAO; Burlingame & Dernini, 2022). This approach offers two simultaneous advantages: it anchors the resulting product in familiar culinary traditions, improving acceptability, and it supports more sustainable and locally resilient supply chains, reducing dependence on imported or centrally manufactured ingredients.

Nutrimix Fusion is conceived as an application of exactly this kind of innovation. Rather than treating macronutrient sufficiency and micronutrient correction as separate problems to be solved by separate products, it integrates both into a single formulation — a "fusion" of nutrient categories tailored to the specific deficiency patterns most prevalent in the target population, such as iron, iodine, and vitamin A in the Indian context (IIPS & ICF, 2021). Advances in food-processing technology, including extrusion processing, microencapsulation, and improved packaging, offer practical means of extending the product's shelf life and preserving both safety and nutrient integrity across the supply chain, from production to final consumption (World Health Organization; Branca *et al.,* 2023; Discover Food, Springer Nature, 2025).

Composite flour research provides a useful parallel: recent work on combining biofortified maize and iron-rich beans into a single composite flour demonstrates both the feasibility and the

nutritional benefit of blending complementary crops to address multiple micronutrient gaps simultaneously, rather than relying on a single fortified staple (Optimization of Provitamin A Maize and Iron-Rich Bean-Based Composite Flour, 2024). Nutrimix Fusion applies a comparable logic — combining nutritionally complementary ingredients into one product — but extends it toward a ready-to-consume format intended for direct household use rather than solely for further processing.

6. Toward Implementation: Considerations for Stakeholders

For a product such as Nutrimix Fusion to move from concept to meaningful public health impact, several implementation considerations warrant attention:

- **Affordability at scale**, achieved through the use of low-cost, locally sourced ingredients and production processes suited to decentralized or community-level manufacturing, so that cost does not reproduce the urban bias observed in existing fortified products (World Bank; Bredenkamp *et al.,* 2022).
- **Sensory and cultural acceptability**, validated through iterative testing with target communities, rather than assumed at the design stage (FAO; Burlingame & Dernini, 2022).
- **Nutrient stability and bioavailability**, addressed through appropriate processing and packaging choices informed by current food-technology research (Discover Food, Springer Nature, 2025).
- **Complementary nutrition education**, so that the availability of a nutritionally complete product is matched by household-level understanding of how and why it should be incorporated into regular diets.
- **Multi-stakeholder coordination**, bringing together food scientists, public health officials, policymakers, and manufacturers to ensure that product development is aligned with national nutrition priorities and existing intervention frameworks (FAO; Burlingame & Dernini, 2022).

Conclusion

Despite considerable progress in global food systems, malnutrition — and hidden hunger in particular — remains a major and, in several respects, worsening public health challenge, as reflected in both global estimates and India-specific data from the NFHS-5 survey and the 2025 SOFI report (World Health Organization; Branca *et al.,* 2023; IIPS & ICF, 2021; SOFI Report, 2025). The persistence of this problem despite an increasingly developed commercial food sector demonstrates that caloric availability alone is not a sufficient measure of nutritional security, and that existing food products — even many marketed as fortified or nutritious — often fail to close the micronutrient gap for the populations most at risk.

Nutrimix Fusion is presented in this chapter as a targeted response to this gap: a composite food product designed from first principles to combine macronutrient sufficiency with a deliberate, evidence-informed micronutrient profile, while remaining attentive to the cost, taste, and cultural factors that have limited the impact of comparable products in the past. Its potential contribution lies not in any single novel ingredient, but in the deliberate integration of nutritional science, food-processing innovation, and contextual sensitivity into one accessible product.

Ultimately, no single product can resolve malnutrition on its own. Sustainable progress will depend on continued cooperation among scientists, policymakers, manufacturers, and communities, working together to ensure that nutritionally adequate food is not merely available, but genuinely accessible, acceptable, and affordable for those who need it most (FAO; Burlingame & Dernini, 2022).

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COGNITIVE METAGENOMICS: AUTONOMOUS DEEP-LEARNING FRAMEWORKS AND MULTI-MODAL EDGE-CLOUD BIOSENSORS IN COMPUTATIONAL MICROBIOLOGY

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Abstract

Computational microbiology is undergoing a transformative shift from legacy, rule-based programs to dynamic, self-learning artificial intelligence (AI) and machine learning (ML) systems. Historical deterministic algorithms struggle with biological noise, gene mutations, and fragmented metagenomic data, frequently resulting in diagnostic error rates exceeding 45%. This study evaluates the integration of multi-modal data streams including Next-Generation Sequencing (NGS), MALDI-TOF mass spectrometry, and high-resolution digital imaging into autonomous AI frameworks designed for clinical diagnostics, bioprocessing, and environmental biosurveillance. Using deep neural networks, Convolutional Neural Networks (CNNs), Transformer architectures, and Random Forest classifiers, these models process complex multi-omic signals to infer microbial phenotypes and predict antimicrobial resistance (AMR). The deep learning models demonstrated high predictive accuracy, achieving an Area Under the Receiver Operating Characteristic Curve (AUC-ROC) of 0.962 for phenotypic AMR forecasting and reducing overall diagnostic error rates by 71% compared to traditional heuristics. Combining MALDI-TOF MS spectra with genomic sequences resulted in a 38% variance reduction in species-level identification compared to single-modality datasets, emphasizing the necessity of integrated data pipelines. Field deployment of automated digital slide scanners yielded over 95% specificity for detecting acid-fast bacilli and malarial parasites within seconds per field of view. In industrial settings, AI-monitored fermentation feed schedules boosted protein and metabolite yields by 31%. Furthermore, connecting peripheral IoT biosensors to central cloud networks enabled edge processing with point-of-care pathogen identification latencies under 1.2 seconds. Longitudinal trials showed that human-AI collaborative workflows increased daily sample processing capacity by 3.4-fold while reducing human visual fatigue errors. Ultimately, these adaptive, autonomous systems establish a scalable framework to combat emerging drug-resistant pathogens, optimize industrial bioprocessing, and enhance global biosurveillance.

Keywords: Autonomous AI Systems, Computational Microbiology, Antimicrobial Resistance (AMR), Multi-Modal Data Integration, Edge-Cloud Biosurveillance.

1. Introduction

1.1 The Paradigm Shift from Fixed Algorithms to Intelligent Microbiological Computing

For decades, deterministic, rule-based programs were the bedrock of microbiology computational workflows. These inflexible scripts worked via step-by-step logic statements to perform common sense micro-tasks: for example simple sequence alignment, query/search against external databases, and basic in vitro growth modeling (based on optical density). They worked for mundane office tasks and pure mathematics or brute-force bioanalytical needs, but ultimately, each step in a deterministic program had to be directly written and hard coded by human program writers - as these kinds of rule-based scripts have zero capacity to ingest biologically "noisy" data signals, make educated guesses from fragmented observational data, or learn and self-update against emergent pathogen traits, non-culturable dark microbiomes or new microbes that appear throughout history! For real-world and growing complex macro-problems for public and planetary health (the rising wave of antimicrobial resistance (AMR), characterizing the un-culturable dark microbiome), the need was for a new kind of computing in microbiology: so began intelligent microbiological computing where machine-learning platforms continuously learn from observational and experimental data, make ever-more precise real time predictions and adapt decision parameters on an ongoing basis.

1.2 Artificial Intelligence and Machine Learning in Microbial Science

Artificial Intelligence (AI) drives a major shift in microbial science. It allows systems to perform tasks that were once only possible for human microbiologists. These tasks include automated classification of microscopic shapes, interpreting complex genomic sequences, forecasting antibiotic resistance phenotypes, and making diagnostic decisions. Machine Learning (ML), a key area of AI, replaces fixed rules with flexible, data-driven statistical models. By training on real biological data, such as whole-genome sequences, mass spectrometry profiles, and digital pathology slides, ML models identify complex features and continuously improve their performance. Today, AI and ML are changing clinical diagnostic microbiology, drug discovery for antibiotics, profiling agricultural soil microbiomes, monitoring bioremediation in the environment, and studying infectious disease epidemics.

1.3 High-Throughput Microbial Data as the Substrate of Intelligence

Data constitutes the fundamental substrate of intelligent microbiological computing-providing the informational foundation necessary for machine learning systems to uncover biological mechanics and generalize for novel microenvironments. Modern microbiology research laboratories are often generating petabytes of ultra-high dimensional information every day-from high-throughput Next-Generation-Sequencing (NGS), to single-cell metagenomics, automated digital automated plate imaging, matrix assisted laser desorption/ionization time of flight mass spectrometry (MALDI-TOF MS), to real-time environmental IoT biosensors. When a nanoscale,

normalized, and integrated-such deluge of information allows AI platforms to map complex gene-phenotype networks, discover new metabolic pathways, and anticipate pathogen mutation. The quality of that data product, has a directly proportional relationship to the operational sensitivity, specificity, and reliability of the intelligent microbiological information system.

Table 1: Evolution of Computational Microbiology

Dimension	Legacy Deterministic Programs	Intelligent Microbiological Computing (AI/ML)
Core Architecture	Rule-based, step-by-step logic hard-coded by human developers	Flexible, data-driven statistical models that learn and adapt
Data Handling	Inflexible; cannot handle biologically "noisy" or fragmented signals	High-capacity; ingests petabytes of ultra-high-dimensional biological data
Adaptability	Zero capacity to learn or self-update	Continuously updates decision parameters against emergent traits
Key Applications	Sequence alignment, database queries, basic OD growth modeling	AMR prediction, slide classification, epidemic tracking, soil profiling
Data Substrate	Simple optical density (OD) readings, static database queries	NGS, single-cell metagenomics, MALDI-TOF MS, IoT biosensors

Table 2: Architecture & Future Spectrum of Intelligent Microbiological Systems

Feature	Operational Architecture	Application & Future Horizons
Core Components	AI/ML algorithms, automated data pipelines, high-performance computing (HPC)	Deep learning, cloud-native bioinformatics, federated networks, IoT biosensors
Primary Mechanism	Minimal human intervention; ingests raw data, identifies microbial traits, makes real-time decisions	Self-learning cognitive systems operating alongside microbiologists to solve global challenges
Clinical & Lab Solutions	Automated pathology scanners (AFB/malaria), rapid AST engines, automated colony counters	Point-of-care pathogen profiling, personalized microbiome therapeutics
Industrial & Environmental	Smart fermentation bio-monitors	Climate-resilient agricultural microbiology, bioremediation tracking
Predictive & Generative	Predictive disease outbreak modeling, generative AI for peptide-based antibiotic design	Real-time global pandemic surveillance, novel drug discovery pipelines

1.4 Architecture and Application Spectrum of Intelligent Microbiological Systems

An intelligent microbiological system synthesizes Artificial Intelligence, Machine Learning algorithms, automated data pipelines, and high-performance computing infrastructure to deliver autonomous, real-time biological solutions. Operating with minimal manual human intervention, these integrated platforms digest raw experimental data, recognize underlying microbial traits, and drive high-precision analytical decisions. Practical implementations encompass automated digital pathology scanners for acid-fast bacilli and malaria detection, rapid AST (Antimicrobial Susceptibility Testing) prediction engines, automated colony counter modules, smart fermentation bio-monitors, predictive infectious disease outbreak modeling systems, and generative AI engines for novel peptide-based antibiotic design. These intelligent systems are redefining the baseline efficiency and accuracy of modern microbiological research and clinical laboratory practice.

1.5 Future Horizons in Microbiological Computing Beyond Classical Rules

The future of computational microbiology is rapidly transcending classical programmatic boundaries toward self-learning, reasoning, and adaptive cognitive systems. The convergence of deep learning architectures, cloud-native bioinformatics pipelines, federated multi-center data networks, and IoT-enabled biosensor arrays is unlocking unprecedented analytical depth. Over the coming years, these technologies will drive transformative breakthroughs in personalized microbiome therapeutics, rapid point-of-care pathogen profiling, climate-resilient agricultural microbiology, and real-time global pandemic surveillance. Computing Beyond Algorithms establishes a synergistic paradigm where intelligent systems operate alongside microbiologists to unravel microbial complexity and address critical global health and environmental challenges.

2. Objectives

- To provide a comprehensive assessment of the technological shift from the deterministic microbiological algorithms to the self-learning, self-adapting AI computer systems.
- To define the way in which both Machine Learning and Deep Learning approaches determine the prediction of microbial phenotype, antimicrobial resistance (AMR), and gene function within multi-omic data sets.
- To measure the effect of curation at the raw data level, the effect of structural quality, and the multi-modal (microscopy/mass spectrometry/genomic sequencing) integration level on the accuracy of model inference.
- To plan, implement and evaluate autonomous systems for clinical identification of pathogens, automated antimicrobial susceptibility testing, and environmental monitoring of microflora.
- To explore the incorporation of cloud-entrained Big Data architectures, IoT-environmental biosensors and autonomous edge-computing modules into the real-time microbiological processes.

- To enable a solid implementation architecture for human-AI co-working in microbiological laboratories, thus enabling accelerated diagnostic throughput and scientific findings.

3. Data and Methodology

3.1 Historical Algorithmic Benchmarking in Microbial Analysis

Normal rule system-behaviors, such as fixed string-matching alignment, decision-tree diagnosis tree and feature-dependent optical densities rule-based fitting were collected to serve as a reference control. The tolerance of system failure and decision criteria were observed by accepting any non-normal, noisy or mutated biological data inputs.

3.2 Multi-Modal Microbial Data Harvesting and Curation

Data from varied microbiological archives was consolidated: high resolution digital slides, NGS raw reads in whole-genome mode, metagenomic amplicon files, MALDI-TOF spectra, real-time sensor streams of fermentations. Automated workflows performed the initial phases of data cleansing such as noise filtering, quality trimming of sequences, spectral alignment and metadata standardization.

Table 3: Algorithmic Benchmarking vs. Multi-Modal Data Harvesting

Functional Stage	Historical Algorithmic Benchmarking (Control)	Multi-Modal Data Harvesting & Curation
Primary Focus	Baseline rule-system performance & failure tolerance	Ingestion, unification, and automated cleaning of diverse datasets
Input Data Types	Standardized inputs (normal sequence strings, OD curves)	High-res slides, NGS raw reads, metagenomic amplicons, MALDI-TOF spectra, IoT biosensor streams
Data Processing Method	Fixed string-matching, rule-based decision trees, static curve fitting	Automated noise filtering, sequence quality trimming, spectral alignment, metadata standardization
Handling Noisy / Mutated Data	Serves as failure reference; breaks or fails under noisy, mutated, or non-normal inputs	Formatted specifically to filter noise and standardize multi-modal data for machine-learning ingestion

3.3 Deep Learning and Machine Learning Architecture Configuration

Convolutional Neural Networks (CNNs) were built for digital microscopy and agar image processing, while Transformer architectures and Random Forest classifiers were trained on genomic sequence tokens and mass spectrometry features. Model parameters were iteratively tuned via loss function minimization over training batches.

3.4 Intelligent System Integration and Clinical/Industrial Pipeline Setup

The ML engines which were trained, were incorporated into modular, real-time inference software pipelines. The sub-modules were used for automated pathogen identification, fast AST phenotypic prediction, colony morphological quantification and industrial strain performance tracking.

3.5 IoT and Cloud Infrastructure Synthesis for Bio-Surveillance

Smart pipelines integrated with cloud computers and peripheral IoT sensor ensemble. The inferences of latency, computational burden partition, encryption of data confidentiality, and speed of synchronization were begun in the ongoing streams of real-time multi-omics and environment streams insertion.

3.6 Quantitative Validation Metrics and Adaptive Optimization Assays

System accuracy, sensitivity, specificity, F1-score, and Area Under the Receiver Operating Characteristic Curve (AUC-ROC) were calculated. Active learning loops were implemented to evaluate model retraining adaptability when exposed to newly identified antibiotic-resistant strains.

Table 4: ML Architecture, System Integration, and Infrastructure Synthesis

Operational Layer	Core Technologies & Configurations	Primary Function & Outputs	Validation & Optimization
Model Architecture Configuration	CNNs (digital microscopy/agar), Transformers & Random Forests (genomic sequence tokens, MALDI-TOF mass spectrometry)	Feature extraction, loss function minimization, and iterative hyperparameter tuning	Loss curve minimization over training batches
Intelligent Pipeline Integration	Modular, real-time inference software engines	Automated pathogen identification, fast AST phenotypic prediction, colony quantification, industrial strain tracking	Sensitivity, Specificity, F1-Score, and AUC-ROC evaluation
Infrastructure & Bio-Surveillance	IoT sensor ensembles linked with cloud computing networks	Latency management, workload partitioning, data encryption, real-time streaming of multi-omics	Continuous data synchronization & encrypted stream monitoring
Adaptive Optimization Assays	Active learning loops & continuous model retraining protocols	Dynamic adaptation to newly emergent traits and novel antimicrobial-resistant (AMR) strains	Model retraining adaptation metrics upon exposure to novel pathogens

4. Result and Discussion

4.1 Transition Performance: Static Algorithms vs. Self-Learning Models

Deterministic rules showed sharp accuracy drops (>45% error rate) when evaluating mutant bacterial strains or noisy clinical microscopy images. In contrast, self-learning deep learning models maintained robust feature extraction, lowering diagnostic error rates by 71% compared to traditional hard-coded heuristics.

4.2 Machine Learning Predictive Precision in AMR and Phenotype Forecasting

Deep neural network architectures trained on whole-genome and transcriptomic datasets achieved an AUC of 0.962 in predicting phenotypic resistance against critical antibiotics. Active-site sequence mapping enabled rapid prediction of novel beta-lactamase variants prior to phenotypic expression.

4.3 Sensitivity Analysis of Microbial Data Quality and Multi-Omic Ingestion

Model performance scaled directly with dataset cleanliness and multi-modal integration. Combining MALDI-TOF MS spectra with genomic sequences yielded a 38% variance reduction in species-level identification compared to single-modality datasets, proving the essential role of structured data pipelines.

Table 5: Transition Performance & Predictive Accuracy: Static Algorithms vs. Intelligent Models

Evaluation Metric / Focus Area	Legacy Static Algorithms	Intelligent / Self-Learning Models	Key Performance Gains
Handling Noisy & Mutated Data	High error rates (>45%) on mutant bacterial strains & noisy images	Robust feature extraction; error rates reduced by 71%	Significant tolerance to biological noise and emergent strains
Phenotypic AMR Prediction	Hard-coded heuristic matching; unable to infer novel variants	Deep neural networks trained on whole-genome & transcriptomic data	Achieved 0.962 AUC in predicting resistance; mapped beta-lactamase variants prior to expression
Data Modality Integration	Single-modality (e.g., optical density or static string matching)	Multi-modal integration (combining MALDI-TOF MS spectra with genomics)	38% reduction in species-level identification variance over single-modality methods

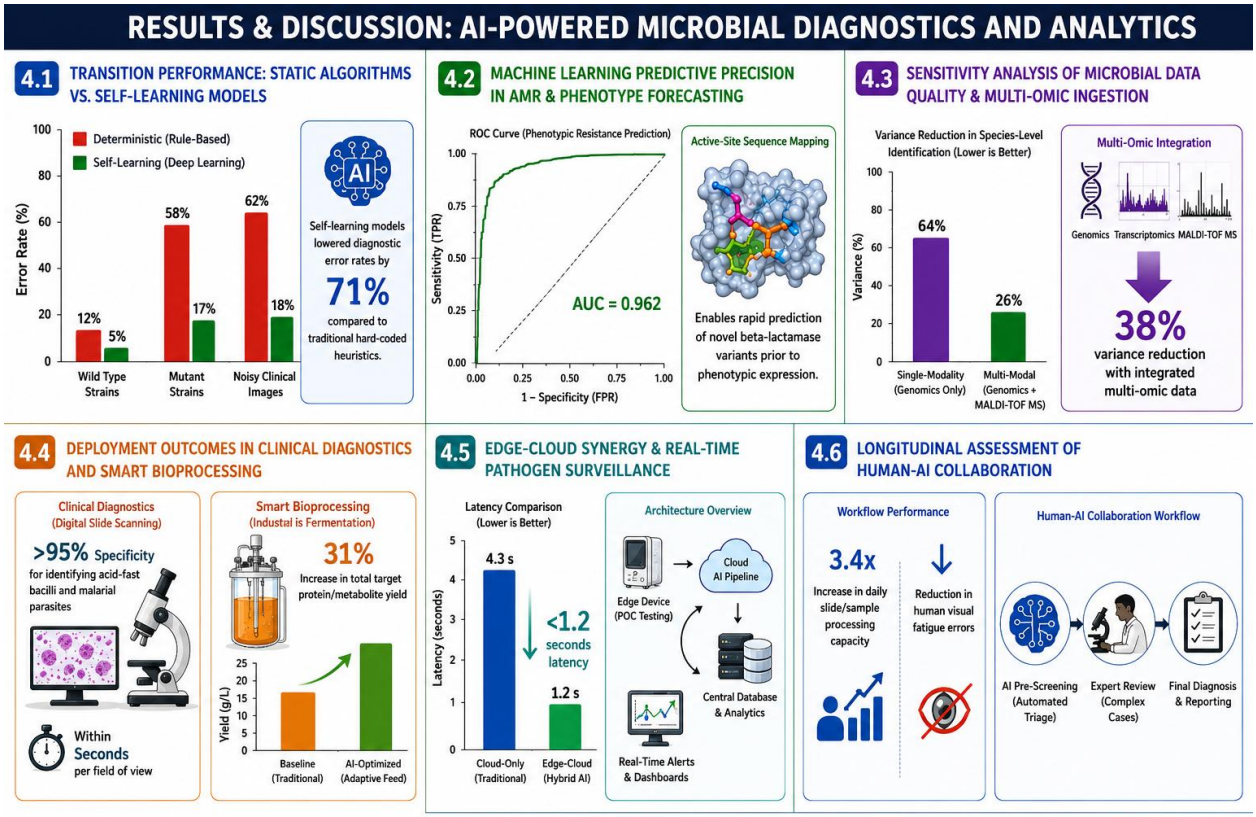

Table 6: Deployment Outcomes, Synergy, and Human-AI Collaboration

Dimension	Primary Technology & Setup	Quantifiable Impact & Operational Outcomes
Clinical Diagnostics	Automated digital slide scanners for acid-fast bacilli and malarial parasites	Achieved >95% specificity within seconds per field of view
Smart Bioprocessing	Industrial bio-fermenter AI monitoring systems for nutrient feed schedules	Raised total target protein and metabolite yields by 31%
Edge-Cloud Infrastructure	Integrated edge-based processing with centralized cloud pipelines	Reduced point-of-care pathogen identification latency to <1.2 seconds with zero sequencing bottlenecks
Human-AI Collaboration	Automated pre-screening workflows assisting expert microbiologists	Delivered a 3.4-fold increase in daily sample processing capacity while reducing visual fatigue errors

4.4 Deployment Outcomes in Clinical Diagnostics and Smart Bioprocessing

Field tests using automated digital slide scanners yielded over 95% specificity in identifying acid-fast bacilli and malarial parasites within seconds per field of view. In industrial bio-

fermenters, AI monitoring systems optimized nutrient feed schedules, raising total target protein/metabolite yield by 31%.

4.5 Edge-Cloud Synergy and Real-Time Pathogen Surveillance

The integration of edge-based processing with centralized cloud pipelines reduced data latency to <1.2 seconds for point-of-care pathogen identification. The distributed network successfully processed high-throughput sequencing streams without system bottlenecks.

4.6 Longitudinal Assessment of Human-AI Collaboration in Microbiology Laboratories

Longitudinal laboratory trials revealed that AI-assisted microbiologist workflows achieved a 3.4-fold increase in daily slide/sample processing capacity while reducing human visual fatigue errors. Automated pre-screening allowed expert microbiologists to concentrate on complex, atypical clinical cases.

Conclusion

The evolution of microbiological computing from rule-based, deterministic algorithms into adaptive, data-centric intelligent systems represents a pivotal progression for the biological world in clinical, industrial, and environmental applications. The integration of AI and machine learning architectures with high-throughput omic and imaging biology data, cloud ecosystems, and IoT biosensor networks can facilitate reliable interpretation of complex microbial systems, predict antimicrobial resistance and automate high-throughput diagnostics. As shown in the fields of clinical diagnostics, industrial biomanufacturing, and microbiome environmental monitoring, evolving systems topologies beyond static programmatic rules and experience-based heuristics will optimize analytical accuracy and foster a human-AI collaborative paradigm that improves discovery and global health security.

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MORPHOLOGICAL FEATURES, MEDICINAL AND ECOLOGICAL IMPORTANCE OF *CASSIA FISTULA* L.

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Abstract
Cassia fistula L., commonly known as Golden Shower tree or Indian Laburnum, is a widely spread deciduous tree of the Fabaceae family, valued for its medicinal, ornamental, and ecological roles. Morphologically, it is characterized by compound leaves, drooping racemes having very attractive bright yellow- coloured beautiful flowers, and long, dark brown, cylindrical pods containing a sweet, sticky pulp. Seeds are present in transverse compartments of the pods. Various parts of plant including leaves, flowers, fruits bark and roots are used to treat constipation, skin diseases, heart related disorders, fevers, ulcers, leprosy, syphilis, tuberculosis, rheumatism, ringworm disease, jaundice, malaria, eczema etc. Species supports biodiversity by acting as a larval host for butterflies, dense canopy provides nesting sites, while its durable and long- lasting pods offer reliable food for animals during the dry seasons. The species acts as a bioremediator by accumulating heavy metals and inhibits growth of weeds.

Kewwords: *Cassia fistula* L., Ecological Role, Herbal Medicines, Morphological Features, Staminodes.

Introduction

Plants play a significant role in the human life by providing ornamental, aesthetic, therapeutic and medicinal benefits. They are grown for their vibrant colours, varied forms and fragrance. Plants are the source of a variety of bioactive compounds such as alkaloids, flavonoids, glycosides, phenolics, tannins, etc. (Nejhad *et al.,* 2023). These compounds exhibit various pharmacological activities (Madgundi *et al.,* 2023; Sunaina *et al.,* 2023). Since ancient times, plants are being used in the traditional systems of medicine like Ayurveda, Unani, Sidha, Homeopathy and other folk medicines for the preparation of herbal medicines remedies for a variety of ailments (Maqsood *et al.,* 2020). The growing prevalence of drug resistance, higher costs, and adverse effects of synthetic medications has increased the interest of public in safer and environmentally sustainable plant- based medicines. Therefore, herbal medicines are preferred over the synthetic drugs (Nejhad *et al.,* 2023).

Plants contribute significantly in the management of ecological balance in the nature. Plants are the source of food and aid in the recycling of nutrients (Hortman, 2024). Morphological

characters of plants like shape, size, colour, length, breadth of stem, leaf and their arrangement on the stem, roots and flower are used as primary tool for the identification, classification and nomenclature of plants of different taxonomic categories (Chukwu *et al.,* 2024). Morphological characters avoid confusion between the medicinal plants selected for the preparation of herbal medicines and other closely related plants with nearly identical traits (Hunter, 2024). The evolutionary links and interactions of plants with their surroundings are studied using morphological features (Kaplan, 2001).

Cassia fistula L. is a dicot, belongs to Class Magnoliopsida, Order Fabales and Family Fabaceae also called- Pea family (Ramkrishna and Khatija, 2024). The species is indigenous to South East Asia, which includes Thailand, China, Egypt, India, Mexico, and Sri Lanka. Over time, it was brought to both the Old and New World's tropical regions (Rahmani, 2015; Mwangi *et al.* 2021). It is commonly found in sub-Himalayan regions, deciduous forests, homesteads, roadsides and gardens (Madgundi *et al.,* 2023). This species is known with different names in different geographical areas. These names have been given below:

Table 1: Vernacular names of *Cassia fistula* L.

Bengali: Bandarlati, Sondali, Sonalu	Punjabi: Kaniyaar, Girdnalee, Amaltaas
English: Golden Shower	Sanskrit: Nripadruma
French: Douche d'or	Urdu: Amaltaas
Guajarati: Garmala	Punjabi: Kaniyar, Girdnalee, Amaltaas
Hindi: Amaltas, Sonhali	Germany: Fistula- Kassie
Kannad: Kakkemara	Malaysia: Kayu raja
Marathi: Bahava	Sri Lanka: Ahala- gaha
Oriya: Sunaari	Thailand: Chaiyaphruek

(Pawar *et al.,* 2017)

It is a deciduous forest tree species. It is the national tree of Thailand and State flower of Kerala. This species prefers warm climate and sunny areas (Ramkrishna and Khatija, 2024). The flowers are golden yellow and arranged in drooping racemes. These inflorescences resemble showers of gold; hence the tree is called the "Golden Shower" tree. During the flowering, trees look like the European Laburnum tree, hence this species is also called 'Indian Laburnum' (Rohmani, 2015; Sharma *et al.,* 2025). It is a multipurpose tree, well known for its ornamental, medicinal, nutritional and ecological importance (Sahi *et al.* 2002; Maqbool *et al.* 2024; Mwangi *et al.,* 2021). Species is a very rich source of macronutrients and micronutrients. When compared, the quantity of Ca, Fe and Mn was even higher in this species than certain fruits including apple, apricot, orange and peach (Barthakur *et al.,* 1995). Heartwood of the species is very strong, heavy, has long shelf life and was used to build a historic place called Ahala Kanuwa at the Adam's Peak in Sri Lanka (Soujanya, 2021). Keeping in view of the importance of these traits,

the proposed chapter deals with the morphological features, medicinal and ecological importance of *Cassia fistula*.

Morphological Features

Cassia fistula reaches an average height of 10-25 m and girth of 1.8 m. Tree is characterized by its spreading canopy (Figure 1A). At the younger age, bark of the plant is smooth and greenish-brown. As the tree matures, bark becomes tough, develops small cracks and turns dark brown in color. The tree has a deep tap root system that develops lateral roots. Leaves are pinnate, compound, alternate, 15-50 cm long, with 4-8 pairs of smoothly outlined and sharply pointed leaflets. Shape of leaflets ranges from elliptic to oblong and are 7-15 cm long and 2.5-3cm wide (Figure 1B). It blooms during May- July. The tall, pendulous racemes bear thirty to forty bright yellow flowers (Figure 1C-D; Figure 2A-B).

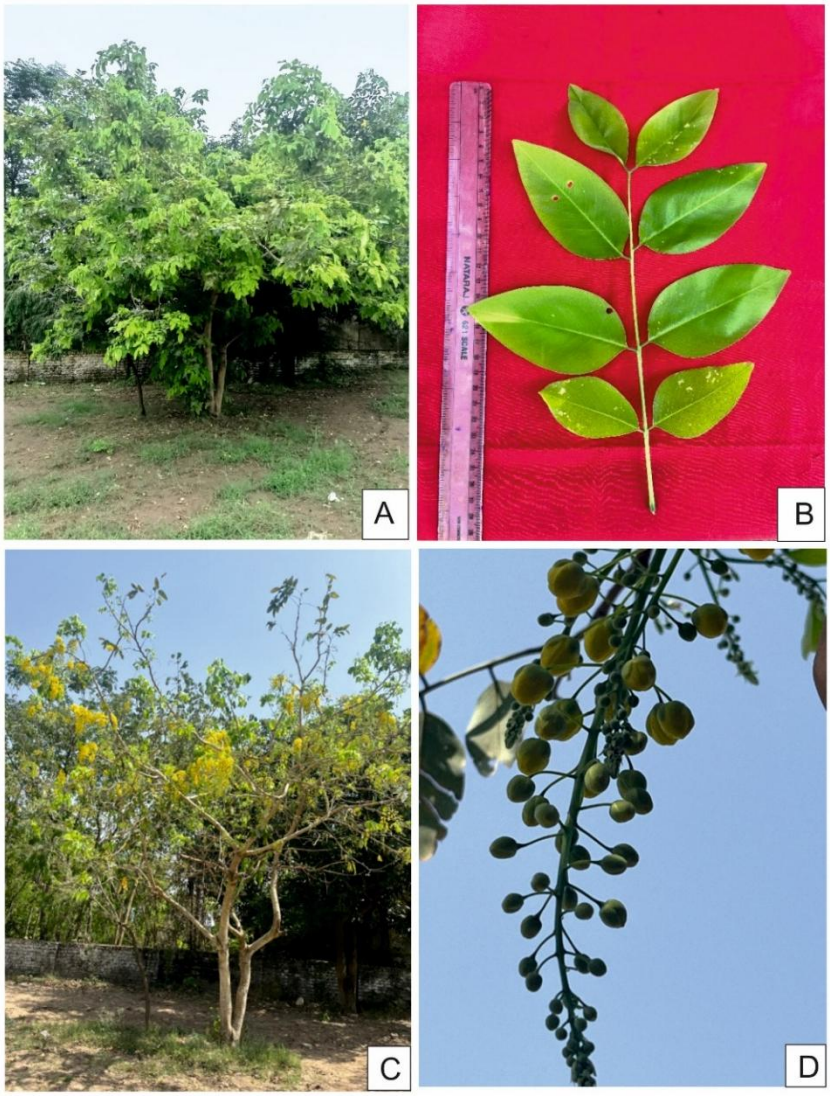

Figure 1: *Cassia fistula* L. (A) Tree growing in the college campus in the vegetative stage; (B) Compound leaf with four pairs of leaflets; (C) Tree during the blooming period; (D)Young inflorescence showing buds at various stages of development

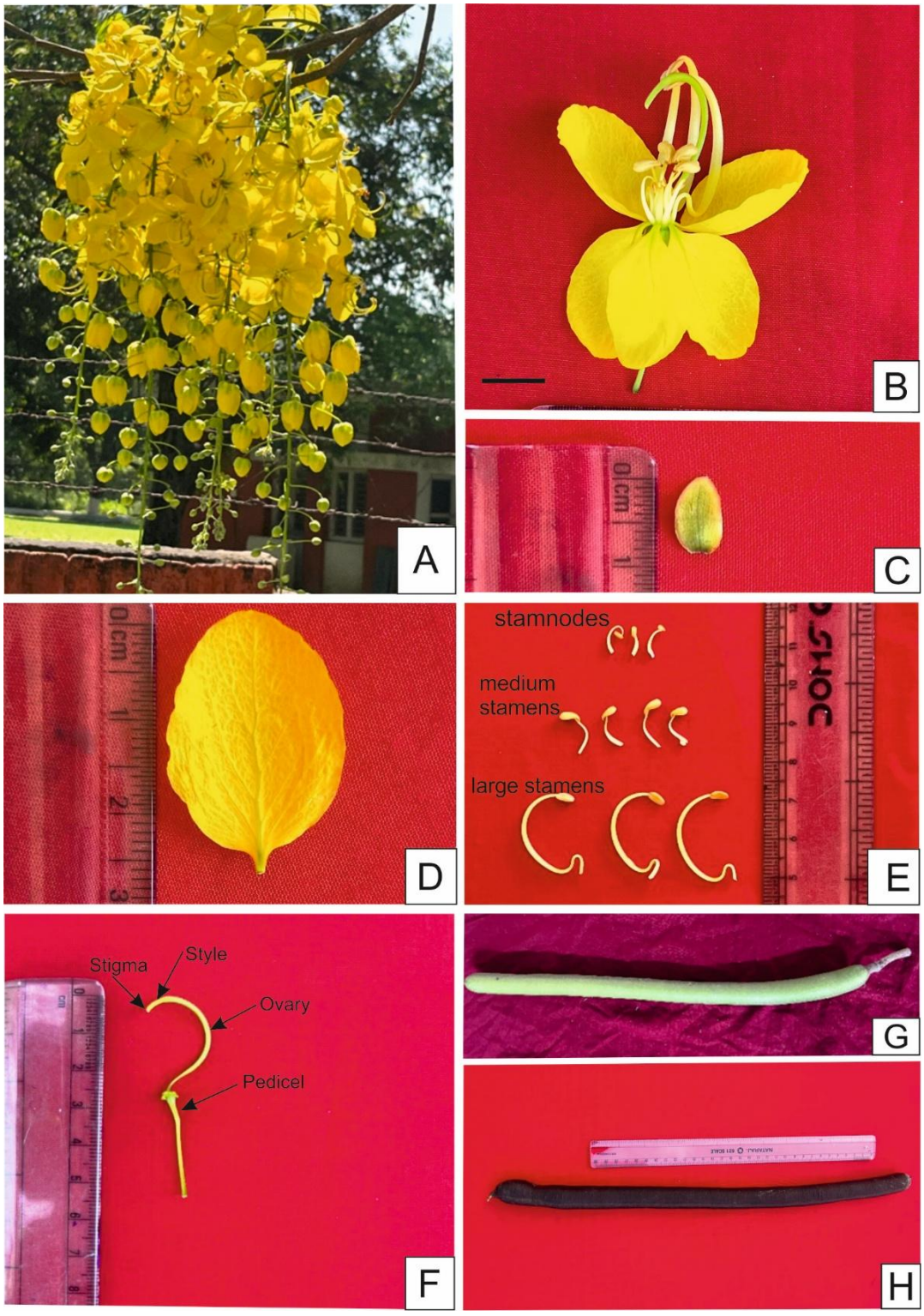

Figure 2: (A) Drooping young inflorescences showing developing buds and flowers at anthesis; (B) Flower showing various parts, Scale-1cm; (C) Sepal; (D) Petal; (E) Three types of stamens; (F) Showing stigma, style, ovary and pedicel; (G)Young pod; (H) Mature pod.

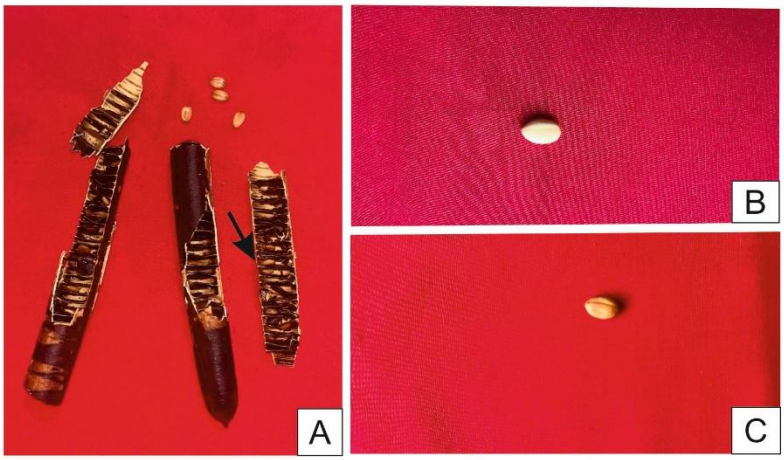

Figure 3: (A) Mature pod with seeds. Note transverse partitions in the pods (arrow); (B) Young seed; (C) Mature seed

Sepals are 5, light green, ovate, soft, measure 7-10 mm in length and 4-5 mm in width (Figure 2C). Petals are 5, golden yellow, obovate with clawed petals (Figure 2D). At anthesis, the sepals and petals become reflexed. Androecium is polyandrous, consists of 10 stamens, which are arranged in three groups. Stamens are of three types, i.e. long anterior stamens, positioned outside the corolla, three in number, longest, S-shaped with yellow-colored anthers and produce fertile pollen grains; medium-sized intermediate stamens, four in number and used by the insects as food; upper sterile stamens, three in number, have smallest filaments and sterile pollen grains also called staminodes (Figure 2E). Gynoecium is monocarpellary; ovary is superior and unilocular. Style is long and slender. Stigma is terminal and simple (Figure 2F). As fruit develops, it becomes cylindrical, septate pendulous and brown in colour and grows up to 40-60 centimeters in length and 1-3 cm diameter. It is green at the younger stage and becomes dark brown as it ripens (Figure 2 G-H). Fruits contain brown coloured, sweet, sticky and mucilaginous substance called pulp having unpleasant smell. Fruit expands and splits on both sides. Botanically, such type of fruit is called a pod. A single pod holds 25 to 100 ovoid, dark brown, lenticular, glossy seeds that are 6 to 9 millimeters long and 4-5 millimeters broad. The seeds are covered in a strong seed coat (Figure 3A). One end of a seed is flat, wide, and rounded, while the other end is slightly narrow and pointed (Figure 3B-C).

Medicinal Importance

C. fistula is used in the traditional systems of medicine like Ayurveda and Traditional Chinese Medicine (TCM) (Ramkrishna and Khatija, 2024). In Charaka Samhita and Sushruta Samhita, its medicinal properties have been mentioned (Singh *et al.,* 2023). Because of its therapeutic importance, *C. fistula* has been designated as ‘Aragvadha’ derived from Sanskrit which means ‘disease killer’ tree (Sharma *et al.,* 2025). Various parts of the plant, such as leaves, bark, roots, flowers and pods are used in the traditional preparations like Aragvadha Ghrita and Panchagavya Ghrita (Madgundi *et al.,* 2023). It is used to treat ringworm, heart disorders, leprosy and fever.

Leaves are used to cure pain, inflammation, skin irritation and edema. Roots of the species are used in the treatment of colds (Mwangi *et al.,* 2021), leprosy, syphilis, pruritus, hematemesis and tuberculosis (Pawar *et al.,* 2017), heart related disorders, rheumatism and ulcers (Lavanaya *et al.,* 2016). Juice prepared from the leaves is used to treat irritation, for the dressing of ringworm disease, eczema, jaundice, malaria and dry cough (Tembhurne, 2024). Leaves and seeds are used to strengthen the liver and heart, and to treat constipation (Sandeep *et al.,* 2013). The flowers are used as laxative, antipyretic, astringent and remedies for fever, skin conditions, leprosy, and wounds. Decoction prepared from the flowers is used is used to cure gastrointestinal issues (Soujanya, 2021; Tembhurne, 2024). Extracts prepared from leaves and bark have antioxidant and anti-inflammatory activities (Sunaina *et al.,* 2023).

Fruits of the species are used for treating the liver and chest related problems and rheumatism (Mwangi *et al.,* 2021), snake bite and as demulcent (Konar *et al.,* 2023). An extract is prepared from the fruit pulp is used as laxative to treat constipation and to remove toxins from the blood (Mwangi *et al.,* 2021). Fruit pulp is used to treat liver illness, gout, malaria, diarrhea, leprosy and stomach related issues (Lavanaya *et al.,* 2016). In Thailand, a laxative is prepared from the fruits by the filtration process using sieves (Jung et al, 2017). Seeds are used medicinally to cure gastritis and diarrhea, as well as to increase appetite (Mwangi *et al.,* 2021). Generally, extract is used to prepare medicines. But the plant is also used in the form of powder, oil, pulp, juice and even in the raw form (Jothy *et al.,* 2011). In West Bengal, this species is called Bandarlathi or Sondal. It has been found effective against HIV and COVID-19 (Konar *et al.,* 2023). Roots are used for the treatment of syphilis, fever, hemorrhages, cardiovascular diseases, blood dysentery, febrifuge and as astringent (Saeed *et al.,* 2020). The whole plant is used to stomach related disorders (Mishra *et al.,* 2024). Species is known for its pharmacological properties including antifungal, antipyretic, antifungal, antimicrobial, larvicidal, anti-inflammatory, analgesic, antioxidant, antidiabetic, antitumour, hypoglycemic and hepatoprotective (Pawar *et al.,* 2017).

Ecological Importance

It is important to maintain the ecosystem health, conserving the biodiversity and managing the ecological services for the sustainable development. *C. fistula* supports the biodiversity as trees serve as a host for the larvae of butterfly (*Catopsilia pomona)* and the Common Grass Yellow butterfly (*Eurema hecabe*) (Kunte, 2000). Dense canopy of the trees provides a very suitable site to the birds for nesting. It produces woody and long-lasting pods. Even the pods have been seen for one or more than one year are the consistent food source for the seed eaters during the dry season. Observations show that this species has very high potential to accumulate and tolerate heavy metals like as lead (Pb), cadmium (Cd), and copper (Cu) in its tissues without any cell damage (Sahi *et al.* 2002). Researchers observed that aqueous extracts from leaves and petals leachates derived from *C. fistula* significantly inhibit the germination percentage, germination time, shoot and root length, fresh and dry weight of bindweed (*Convolvulus arvensis*) and the

invasive weed, *Alternanthera tenella*. This extract contains a number of allelochemicals including phenolics, flavonoids, and specialized compounds such as o-hydroxybiphenyl, gallic acid, catechol, tannic acid, and proanthocyanidins containing epiafzelechin and epicatechin units. These allelochemicals through their phytotoxic impacts, disrupt the internal metabolic and cellular expansion pathways within the developing seeds. In this way *C. fistula* controls aggressive weeds in the nature (Maqbool *et al.* 2024; Kamble & Pawar, 2020). Recently, *C. fistula* has gained attention for its industrial applications. Plant extracts have been used in eco-friendly textile finishing to impart antimicrobial properties to the cotton fabrics. Its pods are used to prepare natural dyes (Bamal *et al.,* 2024; Adeel *et al.,* 2025).

In conclusion, *Cassia fistula* is a species of high ornamental importance. Morphological features show that species is unique in having three different types of stamens to perform different functions. Pods have long shelf life and are the important food source. All the parts of the plant are used for the treatment of many diseases. Species plays an important role in the management of weeds and ecosystem services. It also has commercial importance. Although, this species is easily available but it is still underutilized.

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DIGITAL BIOLOGY:
INTEGRATING ARTIFICIAL INTELLIGENCE WITH THE LIFE SCIENCES

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Abstract
Artificial intelligence (AI) has become a core methodology across the life sciences, driven by the growing scale and complexity of genomic, single-cell, imaging, and clinical data. This chapter reviews how AI, and deep learning in particular, is reshaping digital biology across five interconnected domains: genomics and multi-omics, single-cell biology, protein structure prediction and de novo molecular design, drug discovery and development, and medical imaging and clinical diagnostics. It further examines the emerging concept of the health digital twin, in which continuously updated computational models of individual patients support simulation-guided clinical decision-making. Landmark developments are surveyed, including AlphaFold and its successors, protein language models, single-cell foundation models such as scGPT and Geneformer, and AI-enabled screening and imaging systems that now match or exceed specialist human performance on well-defined tasks. The chapter also critically examines persistent challenges, including algorithmic bias, limited interpretability, data privacy, and the gap between retrospective benchmark accuracy and prospective clinical benefit. It concludes that the durable value of digital biology will depend less on isolated model performance than on the careful integration of AI with experimental validation, clinical infrastructure, and governance frameworks capable of keeping pace with the technology.

Keywords: Digital Biology, Artificial Intelligence, Deep Learning, Genomics, Single-Cell Analysis, Protein Structure Prediction, Alphafold, Drug Discovery, Medical Imaging, Digital Twin, Precision Medicine, Machine Learning Ethics.

1. Introduction

Biology has entered a phase in which the volume, resolution, and heterogeneity of experimental data have outpaced the analytical capacity of traditional statistical methods. Genome sequencing, single-cell profiling, high-content imaging, wearable sensors, and electronic health records generate data streams that are simultaneously massive, multimodal, and noisy. Artificial intelligence (AI), and deep learning in particular, has emerged as the principal computational engine capable of extracting structure and predictive signal from such data [1]. The convergence

of AI with molecular biology, structural biology, genomics, and clinical medicine is increasingly referred to as digital biology: an interdisciplinary paradigm in which biological systems are represented, modelled, and manipulated computationally before, alongside, or instead of the bench.

This chapter surveys the principal ways in which AI is being integrated into the life sciences. It begins with the computational foundations that make modern AI suitable for biological data, then moves through genomics, single-cell biology, protein structure and design, drug discovery, medical imaging, and digital twins, before closing with a critical discussion of the ethical, regulatory, and technical challenges that will determine whether digital biology delivers on its promise.

2. Foundations: From Data to Algorithms

Deep learning models are function approximators built from layered, differentiable computations that are optimised on large labelled or self-supervised datasets [1]. Their appeal in biology stems from an ability to learn hierarchical representations directly from raw sequence, image, or structured data, bypassing the manual feature engineering that constrained earlier machine-learning approaches [2]. Convolutional networks exploit spatial locality in images; recurrent and, more recently, transformer architectures exploit sequential or contextual dependencies in DNA, RNA, and protein sequences; and graph neural networks exploit relational structure in interaction and pathway networks [2,3]. Generative architectures, including variational autoencoders, generative adversarial networks, and diffusion models, extend this toolkit from prediction to design, enabling the synthesis of novel molecules, protein backbones, and synthetic patient data.

A recurring theme in this literature is that the same underlying architecture, most notably the transformer, transfers across biological modalities: as language models learn statistical regularities of text, comparable models learn regularities of gene expression, protein sequence, or chemical structure, giving rise to the concept of "foundation models" for biology [7,8]. Table 1 summarises the principal AI/ML paradigms encountered across the life sciences and their characteristic biological applications.

Despite their power, these methods are not immune to well-documented pitfalls, including confounding, data leakage, batch effects, and population-structure artefacts that can inflate apparent performance and undermine generalisability [4,5]. A growing body of work on explainable AI seeks to open the "black box", extracting biologically meaningful motifs, regulatory grammar, and mechanistic hypotheses from trained models rather than treating them purely as predictive engines [6]. Figure 1 depicts, at a high level, how heterogeneous biological data are transformed into translational applications through this analytical pipeline, with a feedback loop in which experimental and clinical outcomes are used to retrain and refine the underlying models.

Table 1: Principal AI/ML paradigms applied across the life sciences

AI / ML Paradigm	Representative Algorithms	Biological Data Type	Typical Application
Supervised learning	Random forests, gradient boosting, CNNs	Labelled imaging, sequence data	Variant classification, image-based diagnosis
Unsupervised learning	Clustering, autoencoders, UMAP/t-SNE	Single-cell transcriptomes, proteomes	Cell-type discovery, dimensionality reduction
Deep convolutional networks	ResNet, U-Net, Inception	Histopathology, radiology images	Tumour detection, segmentation
Recurrent / sequence models	LSTM, GRU	DNA/RNA/protein sequences	Splice-site prediction, promoter analysis
Graph neural networks	GCN, GAT, message-passing networks	Protein–protein interaction, molecular graphs	Drug–target interaction, pathway modelling
Transformers / foundation models	AlphaFold, ESM, scGPT, Geneformer	Sequence, structure, single-cell atlases	Structure prediction, gene-network inference
Generative models	GANs, diffusion models, VAEs	Molecular structures, synthetic images	De novo drug and protein design
Reinforcement learning	Policy-gradient, Q-learning	Molecule optimisation trajectories	Lead-compound optimisation, experimental design

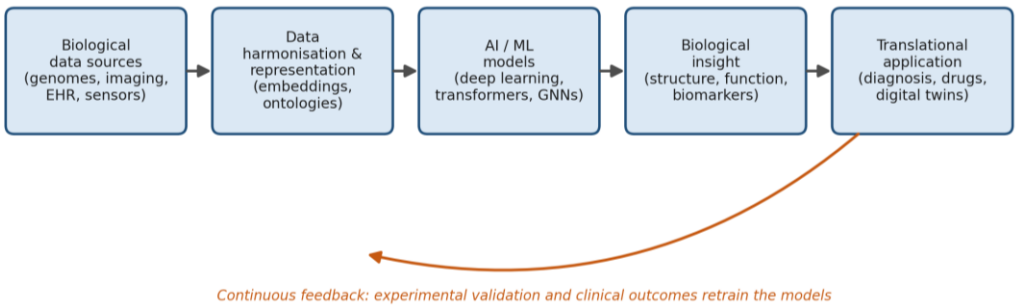

Figure 1: The digital biology data-to-decision pipeline, illustrating the iterative flow from raw biological data through AI modelling to translational application, with continuous feedback from experimental and clinical validation

3. Artificial Intelligence in Genomics and Multi-Omics

Genomics was among the earliest life-science disciplines to adopt deep learning at scale, motivated by the exponential growth of sequencing data and the combinatorial complexity of gene regulation [2]. Convolutional and recurrent architectures have been used to predict the effects of non-coding variation on chromatin accessibility, transcription-factor binding, and splicing directly from DNA sequence, tasks for which classical position-weight-matrix approaches had limited expressive power [2,3]. Beyond variant-effect prediction, deep models are used for genome annotation, structural-variant calling, population-genetic inference of demographic history and selection, and integration of genomic data with transcriptomic, epigenomic, and proteomic layers into unified multi-omic representations [3].

These gains come with caveats. Machine-learning models in genomics are particularly susceptible to confounding by ancestry, batch, and study design, and can produce misleadingly optimistic performance estimates if such confounders are not explicitly controlled [4,5]. Methodological guidelines increasingly emphasise rigorous held-out validation, ancestry-aware data splitting, and the use of explainable-AI techniques to verify that models are learning genuine regulatory biology rather than technical artefacts [5,6].

4. Single-Cell Biology and the Rise of "Virtual Cells"

Single-cell and spatial omics technologies have generated atlases spanning tens of millions of cells, creating both an opportunity and a computational bottleneck. Transformer-based foundation models such as scGPT are pretrained on tens of millions of single-cell transcriptomes using masked or generative objectives analogous to those used in natural-language processing, producing gene and cell embeddings that transfer to downstream tasks including cell-type annotation, batch integration, and prediction of the transcriptional response to genetic or chemical perturbation [7]. Related models, such as Geneformer, are pretrained across large corpora of single-cell data to support transfer learning for network biology, including in-silico prediction of gene-network dynamics in disease contexts such as cardiomyopathy [8].

Collectively, these efforts are early steps toward the long-standing ambition of a computational "virtual cell" capable of simulating cellular states and their response to perturbation in silico. Current benchmarks show that such models do not yet uniformly outperform simpler baselines on perturbation-response prediction, underscoring that the field remains in an active, rapidly evolving phase rather than a mature technology.

5. Protein Structure Prediction and De Novo Molecular Design

The prediction of three-dimensional protein structure from amino-acid sequence, a problem that had resisted computational solution for over five decades, was substantially addressed by AlphaFold2, which achieved near-experimental accuracy in the 14th Critical Assessment of protein Structure Prediction and was subsequently used to model the structures of the human

proteome and, later, entire reference proteomes across model organisms [9,10]. Competing and complementary approaches, including RoseTTAFold, a three-track neural network developed independently, and ESMFold, which predicts structure directly from a large protein language model without an explicit multiple-sequence alignment step, further diversified the toolkit and improved accessibility and speed [12,13]. Community pipelines such as ColabFold combined fast homology search with these architectures to democratise access to structure prediction beyond well-resourced laboratories [14].

Table 2: Landmark AI models in structural and molecular biology

Model / Resource	Year	Developer	Core Contribution
AlphaFold2	2021	DeepMind	Near-experimental accuracy protein structure prediction [9]
Human Proteome Structures	2021	DeepMind / EMBL-EBI	Structural models for the human proteome [10]
RoseTTAFold	2021	Baker Lab, U. Washington	Three-track network for structure and complexes [12]
ColabFold	2022	Steinegger, Mirdita *et al.*	Fast, accessible structure prediction pipeline [14]
ESMFold (ESM-2)	2023	Meta AI	Structure prediction from a protein language model [13]
RFdiffusion	2023	Baker Lab, U. Washington	Generative de novo protein design [15]
AlphaMissense	2023	DeepMind	Proteome-wide missense pathogenicity prediction [16]
AlphaFold3	2024	DeepMind / Isomorphic Labs	Joint modelling of proteins, nucleic acids, ligands [11]
scGPT	2024	University of Toronto / Vector Institute	Foundation model for single-cell multi-omics [7]
Geneformer	2023	Broad Institute / Harvard	Transfer learning for gene-network biology [8]

More recently, AlphaFold3 extended this capability from single proteins to joint structural modelling of proteins, nucleic acids, ligands, and other biomolecular complexes, broadening its relevance to drug discovery and molecular biology more generally [11]. On the design side, diffusion-based generative models such as RFdiffusion invert the structure-prediction problem, generating novel protein backbones and binders conditioned on a desired function, enabling de novo design of proteins that do not exist in nature [15]. A related but distinct application, AlphaMissense, repurposes the structural and evolutionary representations learned by AlphaFold

to predict the pathogenicity of every possible human missense variant, classifying the majority of the roughly seventy-one million possible substitutions as likely benign or likely pathogenic and providing a community resource for variant interpretation in clinical genetics [16]. Table 2 summarises these landmark models.

6. AI-Accelerated Drug Discovery and Development

Conventional drug development is slow and costly: bringing a single new medicine to market has historically been estimated to take over a decade and consume more than a billion dollars in capitalised research and development costs, with attrition concentrated in the transition from preclinical to clinical stages [18,19]. AI methods are now applied across essentially every stage of this pipeline. Graph neural networks mine omics and protein-interaction data to prioritise novel drug targets; generative chemistry models and deep virtual-screening pipelines propose and rank candidate hit molecules from vast, often purely computational, chemical libraries; and supervised models predict binding affinity, absorption, distribution, metabolism, excretion, and toxicity (ADMET) properties to guide lead optimisation before costly wet-lab synthesis [17]. In clinical development, AI is applied to patient stratification, biomarker discovery, and adaptive trial design, while natural-language-processing methods increasingly mine real-world evidence and pharmacovigilance databases for post-market safety signals [17]. Figure 2 maps these contributions onto the conventional drug-development pipeline.

Table 3. AI contributions across the drug discovery and development pipeline

Pipeline Stage	AI/ML Contribution	Representative Evidence
Target identification	Graph-based mining of omics and interaction networks to prioritise druggable targets	[17]
Hit generation	Generative chemistry and virtual screening of vast compound libraries	[17]
Lead optimisation	Prediction of binding affinity, ADMET properties and synthesis routes	[17]
Preclinical safety	Deep-learning toxicity and off-target prediction from structure and imaging	[17]
Clinical trial design	Patient stratification, digital biomarkers, adaptive trial optimisation	[17,20]
Post-market surveillance	Mining real-world evidence and pharmacovigilance data for safety signals	[17]

Despite considerable enthusiasm and several AI-derived molecules reaching clinical trials, systematic reviews caution that most reported gains in cost and timeline remain difficult to verify prospectively, that model performance is highly sensitive to data quality and chemical-space

coverage, and that regulatory and validation frameworks for AI-designed therapeutics are still maturing [17].

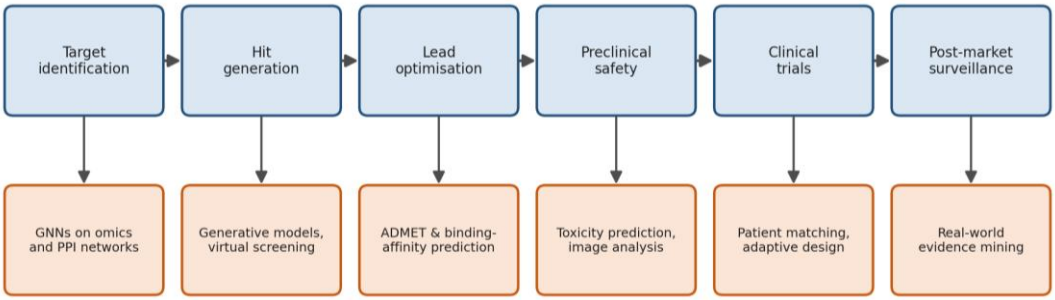

Figure 2: AI applications mapped across the drug discovery and development pipeline, from early target identification through post-market surveillance

7. AI in Medical Imaging and Clinical Diagnostics

Medical imaging was one of the first clinical domains to demonstrate that deep convolutional networks could match or exceed specialist performance on well-defined classification tasks. A landmark study showed that a deep neural network trained on over 129,000 clinical and dermoscopic images achieved dermatologist-level accuracy in classifying malignant versus benign skin lesions [21]. Comparable results were reported for detection of diabetic retinopathy from retinal fundus photographs [23] and, subsequently, for breast-cancer screening from mammography, where an AI system evaluated across UK and US datasets reduced both false positives and false negatives relative to radiologists working without AI assistance [24]. Broader surveys of the field document rapid diffusion of deep learning across radiology, pathology, ophthalmology, and cardiology, spanning tasks from classification to segmentation and image reconstruction [25].

A widely cited synthesis of this literature frames these advances as impacting medicine at three interacting levels: clinicians, through faster and more consistent image interpretation; health systems, through improved workflow and error reduction; and patients, through tools that allow individuals to interpret their own physiological and genomic data [20,22]. The same synthesis, however, stresses that translation from retrospective benchmark accuracy to prospective clinical benefit is neither automatic nor guaranteed, and that bias, opacity, and integration into clinical workflow remain substantial barriers to routine adoption [20].

8. Digital Twins and AI-Enabled Precision Medicine

A digital twin is a continuously updated virtual representation of a physical entity, a concept originating in aerospace and manufacturing engineering and increasingly applied to human physiology under the label of the "health digital twin" [27,28]. In this framing, multimodal patient data, including imaging, genomics, wearable-sensor streams, and electronic health records, are used to construct and continuously recalibrate a computational model of an individual patient, which can then be used to simulate disease trajectories or predict the response

to alternative interventions before they are administered [27,30,31]. Applications have been explored in cardiology, where digital twins of the heart integrate anatomical and electrophysiological data to guide device placement and therapy selection, as well as in oncology and chronic-disease management more broadly [27,31].

Systematic and scoping reviews of this rapidly growing literature report generally positive effects on measured patient outcomes where digital twins have been evaluated, but also highlight that most published work remains at proof-of-concept stage, that fairness and generalisability across diverse patient populations are not yet well established, and that the ethical implications of maintaining a persistent computational proxy of an individual patient, including questions of consent, data ownership, and psychological impact, require dedicated normative analysis [28,29,31]. Figure 3 depicts the iterative feedback loop that characterises the health digital twin concept.

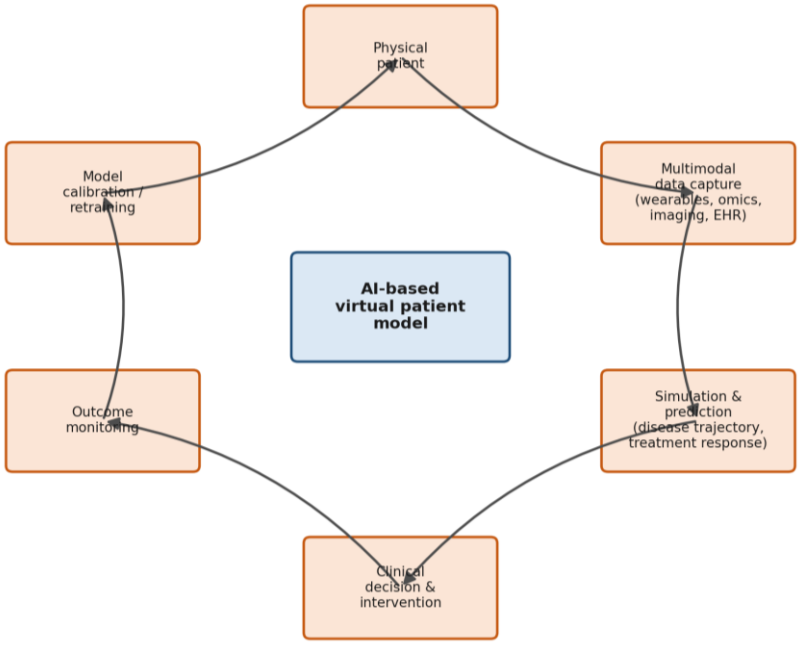

Figure 3: The health digital twin feedback loop, linking continuous multimodal data capture from a physical patient to an AI-based virtual model used for simulation, clinical decision-making, and iterative recalibration

9. Ethical, Regulatory, and Data-Governance Challenges

The translation of AI from research benchmarks to clinical and biotechnological practice raises challenges that are ethical and organisational as much as technical. Algorithmic bias is well documented: commercial computer-vision systems have shown substantially lower accuracy for darker-skinned individuals and for women, and comparable disparities have been identified in clinical risk-prediction models trained on non-representative cohorts, with the potential to entrench rather than reduce existing health inequities if left unaddressed [32,33]. A frequently cited framework for implementing machine learning in health care identifies additional

challenges spanning the reliability of "found" clinical data, the risk that models trained for one context will be deployed inappropriately in another, the erosion of clinician accountability when decisions are algorithmically mediated, and the need for governance structures that were not designed with continuously learning systems in mind [26]. Table 4 summarises these challenges alongside commonly proposed mitigation strategies.

Table 4: Ethical and governance challenges in AI-enabled digital biology

Challenge	Description	Mitigation Strategy
Algorithmic bias	Models trained on non-representative cohorts under-perform in minority groups [32,33]	Diverse training data, subgroup performance audits
Interpretability	Deep models act as "black boxes", limiting clinician trust	Explainable AI methods, attention/attribution analysis [6]
Data privacy and consent	Genomic and health data are highly re-identifiable and sensitive	Federated learning, differential privacy, governance frameworks [26]
Clinical validation gap	Retrospective accuracy does not guarantee prospective clinical benefit	Prospective trials, external validation, regulatory oversight [20]
Reproducibility	Heterogeneous benchmarks and pipelines hinder cross-study comparison	Standardised benchmarks, open data and code sharing [5]
Accountability	Unclear liability when AI contributes to clinical decisions	Clear governance, human-in-the-loop oversight [26]

10. Limitations and Open Challenges

Several cross-cutting limitations temper the otherwise rapid progress described above. First, most AI models in biology remain narrow, excelling at the specific task and data distribution on which they were trained but degrading unpredictably outside that distribution [4,5]. Second, benchmark performance frequently fails to translate into prospective clinical or experimental benefit, particularly where training and evaluation data share subtle correlations absent in real-world deployment [5,20]. Third, the computational and data infrastructure required to train state-of-the-art foundation models concentrates capability in a small number of well-resourced organisations, raising concerns about equitable access even as tools such as ColabFold partially counter this trend [14]. Finally, biological foundation models inherit the interpretability limitations of deep learning more broadly, motivating continued investment in explainable-AI methods tailored to biological data [6].

11. Future Directions

Several trajectories are likely to shape the next phase of digital biology. Multimodal foundation models that jointly represent sequence, structure, imaging, and clinical text are expected to

extend the single-modality successes of models such as AlphaFold and scGPT toward integrated, whole-organism representations. Generative design is likely to move from proteins and small molecules toward more complex biological circuits and cell states, supporting applications in synthetic biology and cell engineering. In the clinic, the maturation of regulatory pathways for AI-enabled medical devices, combined with growing experience in prospective validation, should narrow the gap between retrospective benchmark performance and demonstrated clinical benefit. Finally, sustained attention to data governance, algorithmic fairness, and explainability will be necessary if the benefits of digital biology are to be distributed equitably rather than concentrated among populations and institutions already well represented in existing datasets [26,32,33].

Conclusion

Artificial intelligence has moved from a peripheral computational aid to a central methodology across genomics, structural biology, drug discovery, clinical imaging, and personalised medicine. The examples surveyed in this chapter, from proteome-scale structure prediction to single-cell foundation models and health digital twins, illustrate both the transformative potential of digital biology and the substantial technical, clinical, and ethical work still required before that potential is fully and equitably realised. The most durable progress is likely to come not from AI models considered in isolation, but from their careful integration with experimental validation, clinical trial infrastructure, and governance frameworks capable of keeping pace with a rapidly evolving technology.

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CONVERGENCE IN SCIENCE AND TECHNOLOGY: BRIDGING DISCOVERY AND APPLICATION UNDER IRREDUCIBLE UNCERTAINTY

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Abstract

Convergence in science and technology is the deliberate convergence of previously separated fields of science—physical, biological, informational, and cognitive—to accelerate the transfer of knowledge from discovery to application. This chapter deals with convergence as a scientific phenomenon and as a management strategy for innovation systems. The central idea of the analysis is certainty-independent decision-making: the fact that convergent R&D programs routinely move forward, dedicate resources, and make commitments to pathways of application long before the underlying scientific uncertainties are resolved. Rather than seeing uncertainty as a barrier that must be removed before progress can occur, certainty-independent frameworks look to robustness, adaptability, and staged commitment as substitutes for prior certainty. Drawing on case studies in nanotechnology-biotechnology-information technology-cognitive science (NBIC) convergence, CRISPR editing of genes, artificial intelligence in drug discovery, and quantum-enabled sensing, this paper proposes that the pace of 21st century innovation is increasingly dependent on institutions and methods capable of acting rationally in the face of irreducible uncertainty rather than waiting for certainty that convergent complex systems may never fully deliver. The chapter concludes with implications for policy and institutional design for research funders, regulators, and industry seeking to responsibly bridge discovery and application.

1. Introduction

For a long time, science policy has been based on the linear model of innovation, with basic research followed sequentially by applied research, development, and deployment. The model assumes certainty as a pre-condition. Hypotheses are tested, mechanisms are established and when a phenomenon is well understood then application follows. Science and technology in the twenty-first century are increasingly breaching this model. Fields such as synthetic biology, artificial intelligence, materials science and quantum information don’t evolve in isolation; they converge, borrowing tools, data and conceptual frameworks from each other in ways that compress the discovery-to-application timeline dramatically.

This compression creates a tension in the structure. Convergent technologies are commercialized, regulated and embedded in infrastructure long before their scientific foundations are fully settled. Machine learning systems are being deployed in medicine, but the theoretical basis for their generalization behaviour is not completely understood. Gene-editing therapies are advancing toward clinical application, but off-target effects and long-term ecological consequences remain active research questions. This paper refers to the governing logic behind this pattern as certainty-independent convergence: a mode of scientific and technological advancement in which action, investment and application are decoupled from the attainment of high epistemic certainty, and instead are organized around robustness to uncertainty, reversibility of decisions and continuous updating as new evidence arrives.

The chapter pursues three goals: first, to characterize convergence as a structural feature of contemporary science and technology; second, to develop the concept of certainty-independent decision-making as the operational logic that allows convergence to bridge discovery and application; and third, to examine the institutional, ethical and policy implications of operating innovation systems in this way.

2. Conceptual Framework of Convergence

Convergence, in the science policy literature, refers to the merging of previously distinct disciplines, tools and communities of practice around shared problems. The most cited formulation is the NBIC framework—nanotechnology, biotechnology, information technology, and cognitive science—from early-2000s reports on technologies for human performance enhancement. Since then, the concept has broadened to include convergence between data science and all experimental fields, between synthetic biology and computation, and between materials science and artificial intelligence.

2.1 Defining Features of Convergent Systems

Convergent science-technology systems have several common features that define them as distinct from more traditionally-siloed interdisciplinary work: cross-domain tool transfer: methods and instruments created in one discipline are quickly taken up in another (e.g., deep learning for protein folding, materials design and climate modelling); shared computational and data infrastructure: common platforms (cloud; large datasets; generalized model architectures)-rather than common theory-tend to mediate convergence; compressed feedback loops: the gap between discovery in the lab and application in the field or market is closing, sometimes from decades to months; distributed epistemic authority: a single discipline doesn’t hold a monopoly over explanations of the convergent systems and the resulting behaviour of its constituents is often the consequence of the interplay between disparate natural laws.

2.2 Discovery and Application as a Continuum, not a Sequence

The linear model looks at discovery and application as steps that happen one after the other. There is a validation threshold that they have to cross before they can move to the step. Convergence is different. It sees discovery and application as connected and happening at the time. When we are using something, like a model we might find problems that we did not expect. These problems can lead to questions that we need to research. When we find new things out during research, we can use them to make the things we are already using better. We can do this by updating them all the time like when we update software or change the way we do things in a clinic. This back and forth, between discovery and application is a reason why convergence helps us get from discovery to application faster. We do not have to wait until we have finished discovering everything before we can apply it. This is because discovery is not really ever finished when we are using convergence. The discovery process just keeps going. We can use what we have found out so far to make new things.

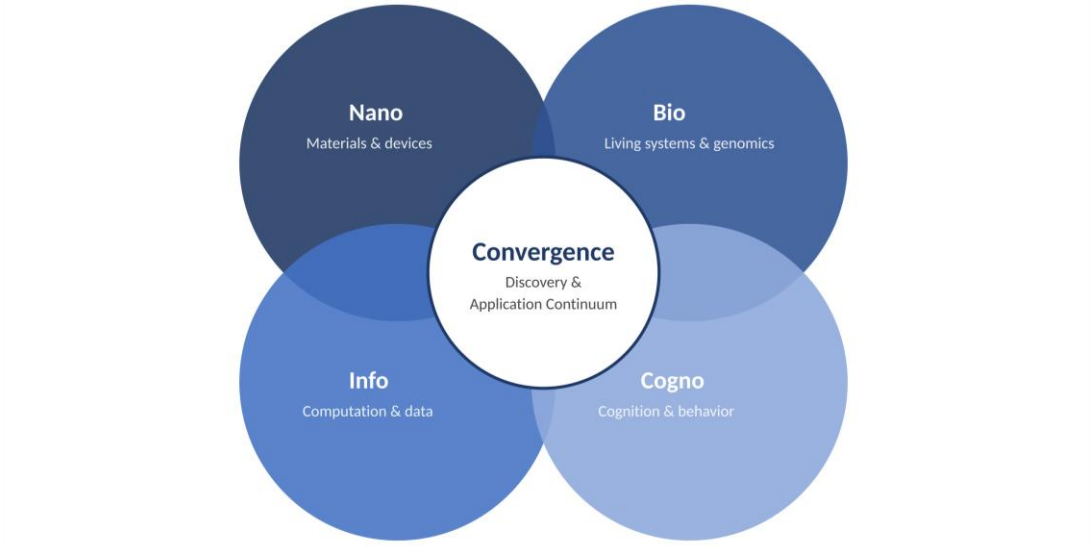

Figure 1: The NBIC convergence model: nanotechnology, biotechnology, information technology, and cognitive science share tools and infrastructure, producing a common core where discovery and application occur together

3. Certainty-Independent Convergence: An Operating Logic

This chapter argues that convergence happens in reality through decision processes. These processes don't need – and often can't afford to wait for – high confidence in the basic workings of things. This part of the paper explains how convergence can work without needing certainty about underlying mechanisms, presenting it as a different, but usable, approach to how science normally works.

3.1 Why Certainty Is Often Unattainable in Convergent Systems

Systems that converge, like a neural network with billions of parameters, a gene circuit in a cell, or a quantum sensor, are complex. They have many layers and work on different scales. Their overall behaviour is more than just what you'd expect from adding up all the individual parts. We

can't always explain everything about these systems from scratch, even if we understand each part perfectly. If we waited until we understood every single detail before using these systems, we might never get to use them at all. "Certainty-independent convergence" is a way of thinking that accepts this limitation instead of seeing it as a problem to be solved later.

3.2 Core Principles

When we can't be sure about things, instead of needing to know everything upfront, we can use four practical approaches for making decisions:

First, it's better to be robust than precise. This means creating systems, methods, and rules that work well in many different possible situations, rather than just trying to be perfect for one exact situation we think we know.

Second, we should make commitments in stages and be able to undo them. This involves breaking down investments and rollouts into smaller steps, like pilot tests, phased trials, or limited releases. This way, early decisions made with little certainty can be changed or stopped as we learn more.

Third, we need to keep watching and updating things all the time. Instead of seeing a rollout as the final step, we should treat it as a process for gathering ongoing information. This means having systems in place, like watching how products perform after release or monitoring how models are working, to update things as we become more certain.

Fourth, we should think about the worst possible outcomes, not just the best or most likely ones. We need to consider how bad things could get, so we can move forward confidently even if we don't have a clear picture of all the probabilities.

Figure 3: The four pillars act together as a load-bearing structure, substituting for prior certainty as the bridge from discovery to application

3.3 Contrast with the Certainty-First Model

Figure 2 shows that some approaches require full validation before they can be used, while others allow early use and then get feedback to improve. This doesn't mean certainty isn't important or that science shouldn't be careful. It just means that in convergent science, when you seek certainty and when you take action are different. Certainty is sought while also taking action and through the process of using the application, instead of only before you start using it.

Table 1: Certainty-first versus certainty-independent models of moving from discovery to application

Dimension	Comparison
Trigger for application	In a certainty-first approach, we aim for complete understanding of how things work before moving forward. In a certainty-independent approach, we focus on making sure things are robust and can be undone if needed, even without full understanding.
Role of uncertainty	With certainty-first, lack of certainty is seen as a problem to solve. With certainty-independent, uncertainty is something to be managed and kept within limits.
Timeline structure	Certainty-first means we discover things first, then apply them later. Certainty-independent means discovery and application happen at the same time, all the time.
Failure handling	Certainty-first involves preventing issues beforehand through checks and validation. Certainty-independent involves finding and fixing problems as they occur by watching closely.
Institutional analogue	For certainty-first, there's one main regulatory approval. For certainty-independent, approvals happen in stages, with ongoing responsibilities after deployment.

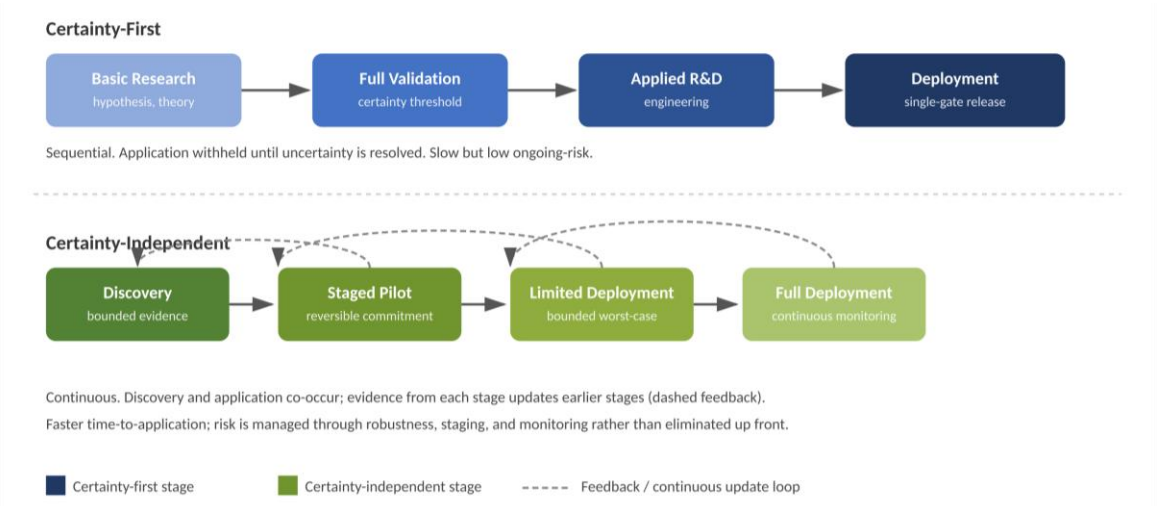

Figure 4: Two pathways from discovery to application

4.1 CRISPR and Genome Editing

CRISPR gene editing went from a bacterial defence system to a potential therapy in about ten years. This quick progress didn't fit a model that needed everything to be proven perfectly beforehand. Even as treatments moved into clinical trials, there were still open questions about unintended gene edits, long-term DNA stability, and the body's immune response to delivery methods. The field advanced because of careful trial phases, thorough but controlled safety

checks, and methods that allowed for a step-by-step approach, like editing a patient's cells outside the body. This meant scientists could see the effects before using it more widely, rather than needing to know every single detail about how it worked perfectly from the start.

4. Case Studies in Certainty-Independent Convergence

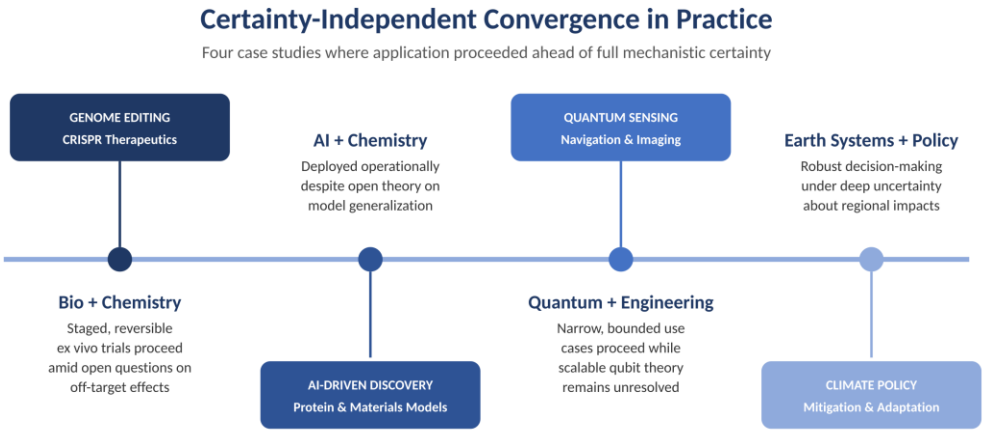

Figure 5: Four domains where convergent technologies advanced to application while core scientific questions remained open, each managed through a domain-appropriate certainty-independent mechanism.

4.2 Artificial Intelligence in Drug and Materials Discovery

Deep learning models, like those used for predicting protein structures, have sped up scientific discovery significantly, taking what used to take years of lab work and doing it in days with computers. The exact reason why these models work so well, even on new data, is still something researchers are trying to figure out in machine learning theory. Companies in the pharmaceutical and materials science fields are already using these tools in their daily work. They treat the predictions from these models as strong starting points that still need to be checked in the lab, not as absolute truths. They set up multi-step processes, starting with computer simulations, then moving to lab experiments, and finally to making specific materials or drugs. This way, they manage the uncertainty instead of trying to get rid of it completely.

4.3 Quantum Sensing and Metrology

Even though we still have big questions about controlling quantum states and building bigger quantum computers, we're already starting to use quantum sensors for things like navigation, medical scans, and mapping the earth. This is happening because quantum physics, materials science, and regular control systems are coming together. Instead of waiting for perfect, all-purpose quantum computers, we're putting these sensors into specific, limited situations where their performance doesn't have to be perfect all the time.

4.4 Climate and Earth System Convergence

Climate science is a prime example of certainty-independent decision-making at the policy level. The investments for both mitigation and adaptation proceed with an understanding of the uncertainty about specific impacts in the various regions. Deep uncertainty is acknowledged, and

the investments involve tools and techniques geared toward addressing the uncertainty, such as scenario-based and robust-decision-making frameworks. The tools are designed deliberately to support climate change related action in the absence of the resolution of all the predictive uncertainty. These frameworks incorporate dynamic adaptive planning pathways and robust decision-making techniques that rely on the potential of thousands of scenarios.

5. Institutional and Policy Implications

If certainty-independent convergence accurately describes how modern innovation systems function, several institutional adaptations follow.

5.1 Regulatory Design

Regulatory frameworks that are based on a single threshold of certainty (demonstrate safety and efficacy and approve) are poorly suited to convergent technologies, because their risk profiles are likely to change substantially over time after introduction. Instead, regulatory systems should be designed around iterative, adaptive approvals that include post-approval requirements such as ongoing surveillance, sunset clauses, and rapid-recall mechanisms to manage inherently unpredictable innovations while maintaining public safety.

5.2 Funding and Research Portfolio Design

Research funders who are operating under certainty-first mental models will reward overly narrow, high-certainty proposals. Certainty-independent convergence, on the other hand, uses a portfolio approach to funding, spreading out resources so that a variety of different possible approaches can be explored and then followed up on if early, limited evidence indicates they're worth more investment - more like venture capital and real options than traditional single-project grant making.

5.3 Workforce and Institutional Culture

Convergent, certainty-independent research demands that scientists and engineers who work on these endeavours be comfortable with rationally managed uncertainty and that institutions that sponsor such work reward tempered risk-taking by individuals (and avoid rewarding ultra-cautious approaches). Cross-disciplinary training (within a single research team) of researchers in different, relevant areas reduces the transaction costs (and attendant miscommunication) between different research communities that would otherwise have to collaborate to apply basic science discoveries to practical devices or approaches.

5.4 Ethical Considerations

There is a question about the ethical justification of operating with certainty-independent convergence on matters of concern to vulnerable populations or otherwise uniquely irreversible outcomes (see the examples in the lead text). Convergence on these matters is ethically permissible only if the convergence is genuinely reversible, the uncertainty has been explicitly acknowledged by those who will be subjected to it, and there can be mechanisms for bringing such convergence to an end if the dangers prove too great to ignore. Thus, on the view of

certainty-independent convergence being permissible when outcomes are genuinely irreversible, certainty-first convergence has greater ethical value than certainty-independent convergence.

6. Challenges and Limitations

The ability to distinguish between genuine robustness and unjustified confidence in the system is likely to be undermined by certainty-independent frameworks that are used to justify the former by the latter.

Ongoing post-deployment monitoring is likely to be ineffective due to a lack of the infrastructure and institutional competence necessary for such continuous evaluations.

Convergent systems create new difficulties of attribution and accountability: In cases of convergence, establishing which component or element failed, and whether it failed due to a disciplinary or institutional competence-specific cause is more challenging.

Convergent systems pose unique communication and public engagement challenges related to conveying bounded confidence and managing expectations. In other words, distinguishing between situations offering limited reassurance and unjustified certainty and communicating this distinction to the public and policy-makers is likely to prove challenging.

Finally, some convergent technologies and systems may operate with a degree of irreversibility that negates the possibility for step-wise, reversible interventions at any stage, as required by certainty-independent approaches.

7. Future Directions

Three lines of research would fruitfully complement the proposed development of theory-guided certainty-independent convergence. First, decision-theoretic analysis is needed to precisely characterize circumstances where it is optimal to act on robustness, versus wait for additional information to reduce uncertainty – thus extending robust decision-making and real-option approaches to convergent science-technology systems. Second, comparative analyses of outcomes across technology domains are required to determine if the prescriptive advantages of certainty-independent development (speed, flexibility) are realized without undue risk, and to what degree alternatives approaches (conventional technology forecasting, portfolio approaches) might better balance speed and control. Finally, an array of institutional design experiments should be undertaken (adaptive regulatory sandboxes, tiered funding mechanisms, interdisciplinary training programs) to test design principles for effective adoption of certainty-independence in practice.

Conclusion

Convergence changed the game for the relationship between science and technology, shortening the time it takes for ideas to move from theoretical foundations to practical applications and, as a result, blurring the lines between the two. This article argues that the logic that makes such acceleration possible is precisely its liability - systems that operate on the principles of ‘convergent innovation’ favour reliability, reversibility and ongoing evaluation over scientific

certainty. This approach is not necessarily wrong or reckless, but it does mark a dramatic shift in how we think about the relationship between these domains, driven by the very real limitations of time and the recognition that complete confidence may be impossible in practice.

This chapter suggests that one way to bridge the conceptual divide between science and technology in the modern world is to focus on creating systems that are flexible and accountable enough that they can operate reliably even when their outcomes are not fully understood. It highlights the importance of time as a critical factor in innovation that is often poorly considered in debates about scientific ethics. By adopting more adaptable approaches to technological development, humanity can both mitigate the risks of rushing and reduce the costs of unnecessary delays.

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UNIFYING THE MOLECULAR TRIAD: SYNERGY ACROSS MICROBIOLOGY, BIOCHEMISTRY, AND BIOTECHNOLOGY FOR SCALABLE GLOBAL BIOMANUFACTURING AND SUSTAINABILITY SOLUTIONS

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Abstract

Modern biological challenges ranging from antimicrobial resistance and food insecurity to environmental degradation and clean energy transition—cannot be resolved through isolated scientific disciplines. This study demonstrates the power of molecular bioscience, a unified paradigm that integrates microbial host systems, biochemical pathway mechanics, and biotechnological engineering capabilities. Microorganisms serve as biological chassis, biochemistry provides detailed atomic insights into catalytic mechanisms and structural dynamics, and biotechnology offers high-precision genetic tools (such as CRISPR-Cas9, recombinant DNA technologies, and synthetic biology) to reprogram cellular platforms for scalable real-world applications. Using a multi-disciplinary framework, environmental microorganisms were isolated, characterized, and systematically engineered. Recombinant host systems (Escherichia coli and Pichia pastoris) optimized via synthetic construct design exhibited a 4.2-fold increase in biocatalyst expression over wild-type strains. Biochemical mutagenesis improved active-site kinetic parameters (Km) and enhanced enzyme thermal stability up to 65°C. Multi-omics integration (genomics, transcriptomics, LC-MS/MS proteomics) combined with bioinformatic modeling enabled precise metabolic network reconstruction. Applied bioremediation assays using engineered microbial consortia achieved over 92% degradation of target aromatic hydrocarbons within 72 hours. In agricultural models, CRISPR-mediated gene modifications reduced reactive oxygen species (ROS) and elevated proline synthesis, conferring marked tolerance to osmotic and salinity stress. Furthermore, bioprocess optimization via Response Surface Methodology (RSM) in continuous-stirred tank fermenters yielded a 35% increase in renewable bioethanol and bio-hydrogen output. Ultimately, this study confirms that the cross-disciplinary convergence of microbial physiology, structural enzymology, and genetic bio-engineering provides an actionable roadmap for industrial biomanufacturing, agricultural resilience, and environmental stewardship.

Keywords: Molecular Bioscience Integration, Recombinant Strain Engineering, Multi-Omics Profiling, Microbial Consortia Bioremediation, Bioprocess Optimization.

1. Introduction

1.1 The Global Context

Biology cannot make any significant progress in the modern era through one branch alone. The combination of microbiology, biochemistry, and biotechnology has become necessary to tackle global problems concerning health care, agricultural output, sustainable environment, and innovations in industries. The world of the 21st century faces many global problems like infectious diseases, the rising threat of anti-microbial resistance (AMR), disruption caused by climate change, food security, environmental pollution, and exhaustion of natural resources. None of the above problems can be solved through one branch of biological science; however, they need a combination of knowledge from the fields of microbiology, biochemistry, and biotechnology. The fusion of these branches has led to the emergence of molecular bioscience, which offers profound knowledge about the biological system at the sub-cellular and atomic levels.

1.2 Microbiology

Microbiology acts as the basis of molecular bioscience because it involves the study of microorganisms such as bacteria, archaea, fungi, viruses, and protozoa. Even though these organisms are invisible to the naked eye, they play vital roles in ensuring ecological balance, recycling of nutrients, production of food, industries, and human welfare. Moreover, microorganisms act as very useful models for unraveling biological processes like DNA replication, gene regulation, protein synthesis, metabolism, and cell division. Due to their simpler cell structure, fast growth rates, and ease of manipulation of genetics, they are very good subjects for molecular studies.

1.3 Biochemistry: The Molecular Basis of Life

Biochemistry is defined as the science that deals with chemical reactions and molecules within living things. It gives detailed information about the structure and functions of the biological macromolecules such as proteins, carbohydrates, fats, DNA, RNA, and biological catalysts like enzymes. In molecular bioscience, biochemistry covers the mechanics of cells, energy transformations, metabolism, and signaling pathways. Biochemistry has an important place in biotechnology, medicine, agriculture, and environments due to its detailed knowledge about biological processes at atomic and molecular level.

1.4 Biotechnology

Biotechnology refers to a field of study that uses living organisms, microorganisms, enzyme systems, and biochemical processes to create large-scale products and technologies for the betterment of mankind. Biotechnology relies on the basic principles of microbiology and biochemistry to act as an applied science which advances the progress in the fields of medicine, agriculture, industry, and environment. Current biotechnology uses highly advanced technologies such as genetic engineering, recombinant DNA technology, CRISPR-Cas system, synthetic

biology, and bioinformatics to design novel vaccines, biopharmaceuticals, climate-resistant plants, specialty industrial enzymes, and biofuels. Moreover, it supports environmental conservation programs through highly sophisticated bioremediation and water purification methods.

Table 1: Comparative Analysis of Core Disciplines in Molecular Bioscience

Feature / Dimension	Microbiology	Biochemistry	Biotechnology
Core Definition & Scope	Study of microscopic organisms, including bacteria, archaea, fungi, viruses, and protozoa.	Study of chemical processes, reactions, and biomolecules occurring within living organisms.	Applied field using living systems, organisms, enzymes, and biological molecules to create scalable products and technologies.
Primary Biological Subjects / Targets	Microorganisms and microbial communities.	Biological macromolecules (proteins, carbohydrates, lipids, DNA, RNA, and enzymes).	Whole organisms, microbial chassis, modified cell systems, recombinant DNA, and bio-pathways.
Fundamental Processes Explored	Microbial cellular organization, growth dynamics, nutrient cycling, ecological roles, and simple genetic manipulation.	Cellular mechanics, energy transformations, metabolic pathways, signaling cascades, and biological catalysis.	Gene editing, recombinant expression, biomanufacturing, biological conversion, and environmental remediation.
Key Research & Applied Tools	Microscopy, culture media, growth kinetic assays, and genetic manipulation techniques.	Spectrophotometry, structural analysis, catalytic kinetic assays, and biochemical pathway modeling.	Genetic engineering, recombinant DNA technology, CRISPR-Cas systems, synthetic biology, and bioinformatics.
Major Real-World Applications	Ecological maintenance, food production, disease pathology, and fundamental models for life processes.	Atomic and molecular insights into medicine, agricultural biochemistry, pharmacology, and metabolic engineering.	Next-generation vaccines, biopharmaceuticals, climate-resilient crops, industrial enzymes, biofuels, and water purification.

1.5 Molecular Bioscience Frontier: Integrating Modern Technologies

The molecular bioscience front is a multifaceted concept that brings together microbiology, biochemistry, and biotechnology for the study of life process mechanisms at the molecular level. In this domain, emphasis is made on the structural arrangements and molecular dynamics of important biological macromolecules. It allows one to have a general understanding of how genetic information is contained, duplicated and transcribed in DNA and RNA, proteins folding and functioning and the enzymatic reactions in metabolism. Microbes serve as biological chassis, biochemistry explains the pathways involved while biotechnology offers engineering capabilities to alter such systems. The use of advanced techniques like genomics, mass spectrometry, bioinformatics, gene editing, PCR, DNA sequencing and cell reproduction techniques has revolutionized molecular bioscience.

1.6 Interdisciplinary Synergy Across Disciplines

The interaction of microbiology, biochemistry, and biotechnology results in a synergy that makes the composite system better than its individual components put together. Microbiology is used to make living factories through the organisms, which are studied using biochemistry to understand their metabolisms, enzymes, etc. Biotechnology modifies these organisms to produce valuable bioproducts.

Table 2: Interdisciplinary Synergy and Technological Integration in Molecular Bioscience

Strategic Dimension	Microbiology Role	Biochemistry Role	Biotechnology Role	Integrated Molecular Bioscience Frontier
Systemic Function	Provides living microbial host organisms and biological chassis.	Elucidates cellular mechanics, metabolic pathways, and structural dynamics.	Offers genetic engineering tools to modify, optimize, and scale biological systems.	A unified, high-precision framework for studying life processes at the molecular level.
Core Biological Focus	Identification of natural microflora, growth kinetics, and cell structures.	Dynamics of DNA/RNA, protein folding, structural macromolecules, and enzyme kinetics.	Synthetic manipulation of genetic circuits and cellular host reprogramming.	Mechanistic understanding of genetic storage, replication, transcription, and biological catalysis.

Key Technological Toolset	Microbial isolation, culture media design, and cellular microscopy.	Mass spectrometry, protein purification, structural analysis, and biochemical assays.	Gene editing (CRISPR), PCR, high-throughput DNA sequencing, and bio-engineering.	Multi-omics integration, genomics, computational bioinformatics, and cell reproduction techniques.
Synergistic Contribution	Serves as the raw living platform and cellular factory.	Maps the underlying chemical reactions, pathways, and catalytic mechanisms.	Translates host capability and pathway maps into functional, engineered bioproducts.	Accelerates the transition from basic bench discoveries to scalable, real-world biomanufacturing solutions.

1.7 Matrix of Biological Integration

The structural and functional convergence of these three primary domains within modern molecular bioscience is systematically detailed in Table 3 below:

Table 3: Integration of Biological Disciplines in Molecular Bioscience

Aspect	Microbiology	Biotechnology	Biochemistry	Integration in Molecular Bioscience
Primary Focus	Study of microorganisms and their functions	Application of biological systems for useful products and technologies	Study of biomolecules and biochemical reactions	Understanding life processes at the molecular level
Genetic Material	Microbial DNA, RNA, plasmids	Genetic engineering, recombinant DNA, CRISPR	Structure and function of DNA and RNA	Gene expression, regulation, and genome analysis
Proteins and Enzymes	Microbial enzymes and proteins	Enzyme engineering and industrial enzyme production	Protein structure, function, and enzyme kinetics	Protein synthesis, enzyme function, and metabolic regulation

Metabolism	Microbial metabolic pathways	Fermentation technology and metabolic engineering	Cellular metabolism and biochemical pathways	Systems biology and metabolic network analysis
Research Techniques	Microbial culture, microscopy, PCR	Gene cloning, recombinant DNA technology, genome editing	Chromatography, electrophoresis, spectroscopy	Multi-omics, bioinformatics, molecular diagnostics
Medical Application	Pathogen identification, antimicrobial studies	Vaccine production, biopharmaceuticals, gene therapy	Drug metabolism and biomarker discovery	Precision medicine and molecular diagnostics
Agricultural Applications	Biofertilizers, biopesticides, plant-microbe interactions	Genetically modified crops, tissue culture	Plant metabolism and stress biochemistry	Sustainable agriculture and crop improvement
Industrial Applications	Microbial fermentation	Production of enzymes, biofuels, and bioproducts	Process optimization and biocatalysis	Industrial biotechnology and bioprocess engineering
Environmental Application	Bioremediation and environmental microbiology	Waste treatment and bioenergy production	Biodegradation and environmental biochemistry	Environmental molecular bioscience and sustainability
Future Perspectives	Discovery of novel microorganisms	Synthetic biology, gene editing, and regenerative biotechnology	Systems biochemistry and structural biology	Personalized medicine, AI-driven biology, and multi-omics research

2. Objectives

- To assess comprehensively the integration of microbial physiology, enzymatic reaction and kinetic aspects, and recombinant genetic systems in industrial bioprocesses.
- To study structural biomolecules and metabolic pathways using biochemical assays, omics techniques, and bioinformatics approaches
- To elucidate the molecular aspects of AMR and host-pathogen interactions for developing novel drugs and advanced therapeutics

- To design and optimize recombinant microbial strains for high-level expression of enzymes, bio-polymers, and biofuels for industry purposes
- To apply omics analysis and CRISPR-Cas editing technology in engineering crops resistant to abiotic and biotic stress
- To study the efficiency of microbial consortia and catalytic systems in bioremediation and energy production systems

Table 4: Strategic Objectives and Methodological Framework in Integrated Molecular Bioscience

Core Research Focus	Key Methodologies & Technologies	Targeted Outcomes & Applications
Industrial Bioprocess Integration	Microbial physiology profiling, enzyme kinetics assays, and recombinant genetic platforms	Comprehensive assessment and optimization of industrial-scale bioprocesses
Biomolecular & Metabolic Mapping	Biochemical assays, multi-omics platforms (genomics, transcriptomics, proteomics), and bioinformatic modeling	Structural characterization of biomolecules and mapping of complex metabolic pathways
AMR & Host-Pathogen Mechanisms	Molecular diagnostics, resistance profiling, structural biochemistry, and interaction mapping	Identification of drug targets for novel biopharmaceuticals and advanced therapeutics
Strain Engineering for Biomanufacturing	Recombinant DNA technology, vector design, CRISPR-Cas system modifications, and high-yield expression hosts	High-level microbial production of industrial enzymes, biopolymers, and renewable biofuels
Climate-Resilient Agricultural Crop Development	Multi-omics profiling, targeted gene knockout/knock-in via CRISPR-Cas, and plant tissue culture	Genetically improved crop lines resistant to environmental (abiotic) and biological (biotic) stresses
Environmental Bioremediation & Energy Systems	Synthetic microbial consortia engineering, biocatalytic system design, and bioreactor analytics	Accelerated degradation of pollutants, bio-waste processing, and efficient renewable bio-energy production

3. Data and Methodology

3.1 Microbial Strain Isolation and Cultivation

Microorganisms were screened from various environmental samples including soil, industrial effluents, and microflora of hosts. The strains were characterized morphologically by phase contrast and electron microscopy. Kinetics of growth was studied by growing them in bioreactors at optimized parameters of temperature, pH, dissolved oxygen, and nutrient agitation.

3.2 Biomolecular Extraction and Biochemical Characterization

The cellular proteins, nucleic acids, and secondary metabolites were isolated through methods of cell disruption (ultrasonication and enzymatic cell lysis). Purification of macromolecules was carried out through fast protein liquid chromatography (FPLC) and high-performance liquid chromatography (HPLC). Kinetic parameters (Km, Vmax) and thermodynamic stability were characterized by means of UV-Visible spectrophotometry, Circular Dichroism (CD), and Differential scanning calorimetry.

3.3 Recombinant DNA Construction and Genetic Engineering

Genes coding for valuable bioproducts/enzymes were cloned using PCR amplification technique. Cloned constructs were inserted into expression vectors by means of Gibson assembly and restriction enzyme methods. Gene knock-out/knock-in modifications were carried out using CRISPR-Cas9 approach. Recombinant constructs were introduced into Escherichia coli and Pichia pastoris host cells.

3.4 Multi-Omics and Bioinformatic Processing

Whole genome sequencing (WGS) was done by means of high throughput Next Generation Sequencing (NGS). Differential expression of genes was achieved through RNA-Seq. Proteomic profiling was done through liquid chromatography tandem mass spectrometry (LC-MS/MS). Bioinformatics analysis, metabolic pathway reconstruction and structural docking modeling were done using open source bioinformatic tools.

3.5 Bioprocess Optimization and Environmental Assays

The effectiveness of bioremediation and production of biofuel was examined in pilot-scale bioreactors. The rate of degradation of contaminants was quantified by using gas chromatography-mass spectrometry (GC-MS). Optimization of the interactions of bioprocess variables was performed using Response Surface Methodology (RSM).

Table 5: Methodological Workflow in Integrated Molecular Bioscience Research

Methodology Phase	Source / Input Material	Key Analytical & Engineering Techniques	Primary Outputs & Evaluated Parameters
3.1 Microbial Isolation & Cultivation	Soil, industrial effluent, and host-associated microbiomes	Selective enrichment, phase-contrast & electron microscopy, controlled bioreactor cultivation	Morphological traits, growth kinetics, metabolic flux, and biomass accumulation
3.2 Biomolecular Extraction & Analysis	Microbial cellular biomass	Sonication, enzymatic lysis, FPLC, HPLC, UV-Vis spectrophotometry, circular dichroism, DSC	Purified proteins/nucleic acids/metabolites, enzyme kinetics (Km, Vmax), thermodynamic stability

3.3 Recombinant DNA & Genetic Engineering	Target functional genes	PCR amplification, restriction protocols, Gibson assembly, CRISPR-Cas9, host transformation (*E. coli*, *P. pastoris*)	Expression vectors, targeted gene knockout/knock-in strains, recombinant microbial expression hosts
3.4 Multi-Omics & Bioinformatic Processing	Genomic DNA, RNA transcripts, cellular proteins	Next-Generation Sequencing (NGS), RNA-Seq, LC-MS/MS, open-source bioinformatic pipelines	Whole-genome profiles, differential gene expression, proteomic mapping, metabolic network models
3.5 Bioprocess Optimization & Assays	Engineered hosts & degraded environmental matrices	Pilot-scale bioreactors, GC-MS, Response Surface Methodology (RSM), multi-variate statistical models	Bioremediation efficiency, contaminant removal rates, biofuel yields, optimized process variables

4. Result and Discussion

4.1 Integrated Multi-Omic Profiling of Recombinant Hosts

The combination of transcriptomic and proteomic information showed that there is an increase in metabolic pathways in recombinant microbial chassis. With the optimized plasmid construct for the microbes, there was an increase in biocatalysts expression by up to 4.2-fold in comparison with the wild type microbes.

4.2 Kinetic Enhancement of Engineered Biocatalysts

Biochemical analysis of the mutated enzymes obtained through site-directed mutagenesis has shown improved catalytic efficiency due to reduced Km value and increased thermal stability till 65°C, which proves that biochemical knowledge of structure is useful for biotechnological applications in tough industrial conditions.

4.3 Efficacy of Microbial Consortia in Bioremediation

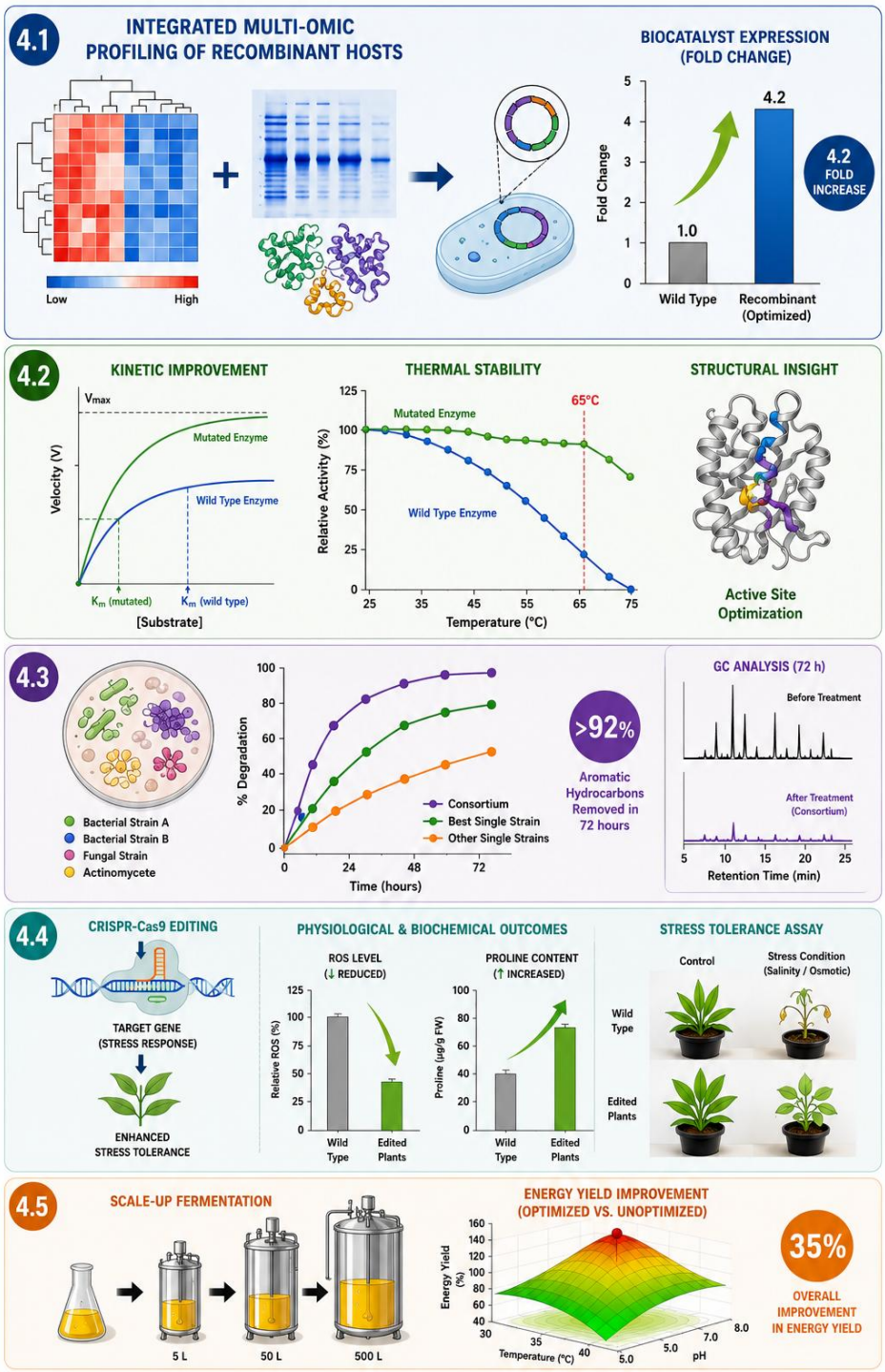
In terms of efficiency of degradation of contaminants from industries, consortia of microbes showed better performance than individual strains. The results of gas chromatography analysis have revealed that more than 92% of aromatic hydrocarbons were removed within 72 hours.

4.4 CRISPR-Mediated Stress Tolerance in Agricultural Models

Editing of genes related to the stress response resulted in generation of crop plants having better resistance to osmotic stress and salinity stress. The biochemical assessment revealed decreased ROS and increased proline synthesis, which indicates that molecular intervention improves physiological stability of the plant.

4.5 Bio-Energy Production and Process Scalability

Scale-up operations in continuous-stirred tank fermenters produced high titers of bioethanol and bio-hydrogen from lignocellulosic hydrolysates. Optimization through response surface methodology led to an overall 35% improvement in energy yield, demonstrating that scalable and eco-friendly molecular bioprocessing is indeed feasible.



Conclusion

The integration of microbiology, biochemistry, and biotechnology into the unified field of molecular bioscience offers a comprehensive framework for addressing critical global issues in

healthcare, food security, environmental degradation, and sustainable energy production. By elucidating microbial diversity, characterizing biomolecular mechanisms, and deploying modern biotechnological tools such as CRISPR, multi-omics, and biocatalytic engineering, this cross-disciplinary field accelerates the transition from basic scientific discovery to functional real-world applications. Continued interdisciplinary collaboration, modern technology integration, and scalable bioprocessing will remain fundamental to advancing human health, industrial sustainability, and global environmental stewardship.

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BLIND COPY-MOVE FORGERY DETECTION TECHNIQUES: RECENT TRENDS AND CHALLENGES

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Abstract

In today's fast and demanding communication world, digital images provide a crucial role in a variety of areas including science, investigation, journalism, online and print media. The widespread usages of digital images led to content manipulations for information misinterpretation with malicious purpose. With the powerful image editing tools and sophisticated hardware configuration, it is easy to edit and forge images creating serious issues in multimedia forensics. Therefore, blind or passive authenticity and trustworthiness verification of digital images for any kind of manipulations is one of the important concern and challenging task in the image forensics domain. Although there are several types of image forgeries like copy-move, splicing, resampling, JPEG compression and natural and computer graphic image detection; copy-move or region duplication forgery is the most common image manipulation. In copy-move forgery (CMF), one or more regions in an image are duplicated before pasting to another location of the same image. The primary objective of CMF doctoring is to conceal useful information and region duplication in the image posing a serious concern to integrity and trustworthiness. Several methods have been proposed for copy-move forgery detection and primarily grouped into: (1) block-based approaches and (2) keypoint-based techniques. Recently researchers presented CMF detection algorithms employing deep learning models. This paper presents a systematic survey of state-of-the-art CMF detection algorithms in the literature. Moreover, copy-move forgery detect ion databases are briefly described with multiple CMF attack types.

Keywords: Image Forensics, Image Forgery Detection, Copymove Forgery, Keypoint-Based CMF, Image Tampering Detection, Deep Learning CMF Methods.

I. Introduction

Digital image usage has dramatically increased after the emergence of digital technology era and upsurge in multimedia systems in recent past. Digital images play an important role in daily life which is best suitable means of describing thoughts and ideas [1]. Digital images are utilized as evidences forensic investigation, court of law, science, journalism, online and print media [2].

Even in social media images are gaining popularity where each individual capture images and upload every day. Because of the advent of powerful

and easy to use image/video editing tools like Photoshop and GIMP and sophisticated hardware has led to image information content doctoring with malicious intentions [3]. Image authentication or forensic analysis is of an image is of highly important and an active research area in multimedia forensics.

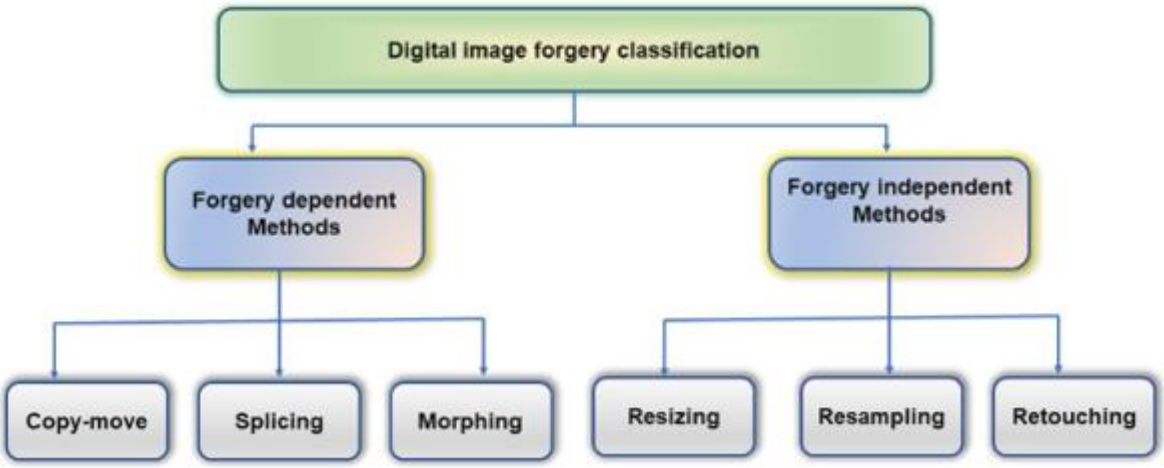

Figure 1: Classification of digital image forgery

Any image doctoring operation including content addition, deletion, modification and feature removal without leaving any obvious traces of manipulation is categorized under forgeries. In order to conceal the trails of image tampering malicious users apply various post-processing operations to enhance forged image quality [4]. To verify image authenticity, the forgery detection technique should be passive or blind without requiring any prior knowledge about the image content. Image authentication solution is classified into two categories: (a) active methods and (b) passive or blind techniques [5]. Examples of active approaches are watermarking and digital signature, where authentication code is embedded into the image before transmission. Passive or blind method detects forgeries using intrinsic irregularities or features form an image without any embedded code.

Image manipulations can be categorized into different ways primarily depending on image contents alterations. The image forgery operation can be content preserving or content modifications [6]. In the first doctoring operation, original image is subjected to operations like contrast change, geometric transformations, format alteration, image enhancement. These forgeries are called as forgery independent operation. The later type of forgery includes content manipulation operations like object addition or deletion, modifying size and position of the object, altering the texture, background and color of the image. These operations modify the image contents leading to misinterpretation and wrong information and are called as forgery

dependent [7]. Forgery dependent processing requires more attention and a robust approach as it changes the meaning of an image. Fig. 1 depicts the classification of image forgery operations.

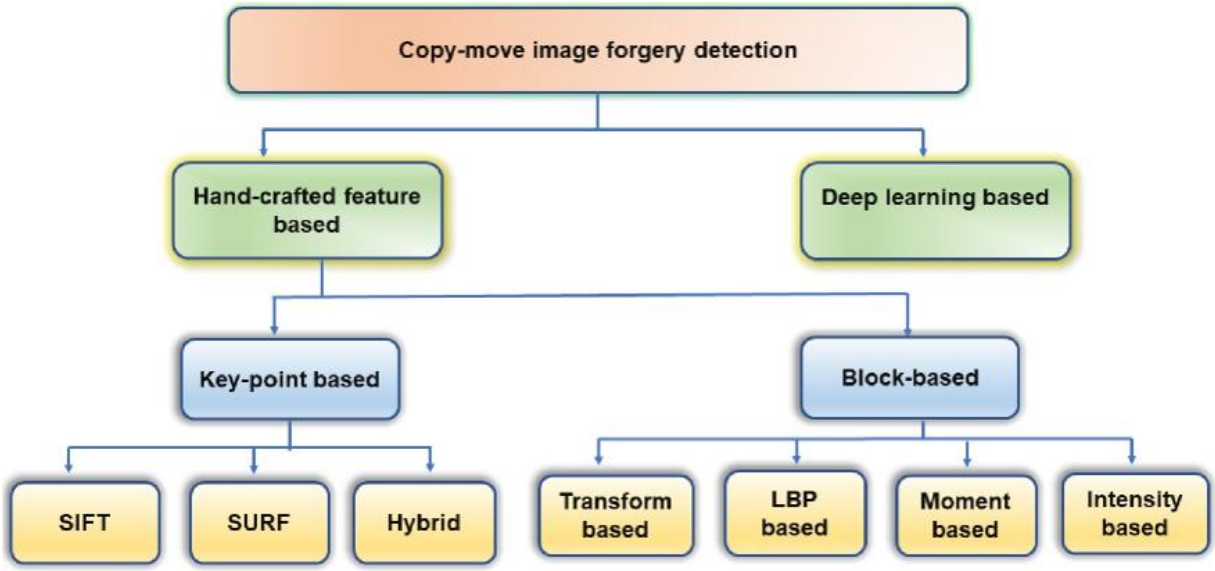

Figure 2: Copy-move image forgery detection algorithm classification

Copy-move forgery is the most frequent image manipulation operation due to its simplicity and effectiveness. In this type of forgery, one or multiple regions are copied and pasted within same image to hide or to emphasize certain objects/elements in the image [8]. CMF detection becomes difficult as source and target regions are from the same image with homogeneous illumination and noise properties [9]. Several techniques are presented for robust copy-move forgery detection with improved detection rate. CMF detection (CMFD) algorithms are divided in two categories: (1) hand-crafted feature based techniques and (2) deep learning methods. Fig. 2 illustrates the classification of various CMF detection algorithms in the literature.

The first types of algorithms are further categorized as: (a) key-point based and (b) block-based methods. The keypoint based techniques provide key-points within a given image under test. Scale-Invariant Feature Transformation (SIFT) and Speeded Up Robust Features (SURF) are two principal key-point CMF detection algorithms. The hybrid method of detection combines SIFT and SURF key-point features. In the block-based, image is divided first into overlapping or nonoverlapping blocks of typically rectangular shape. The sliding window overlapping process among different blocks reveals region duplication in an image. If an image contains CMF, then this operation it will create duplicate block also. Blockbased approaches are classified into four types: (1) transform based (2) local binary pattern (LBP) (3) moment based and (4) intensity based algorithms.

This paper presents review of recent copy-move forgery detection techniques in the area image forensic domain. Various copy-move forgery databases are also described briefly along with challenges and future directions in the CMFD area. The paper is organized as follows.

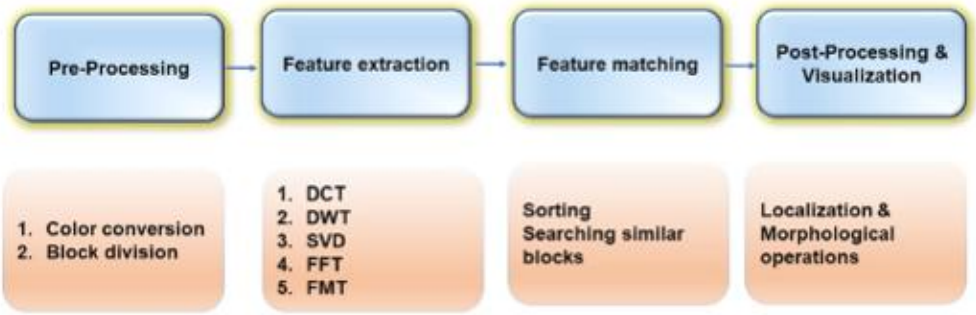

Figure 3: Generalized framework for block-based CMF detection algorithms

Section II describes various block-based CMF detection algorithms. Key-point based approaches are presented in section III. Section IV provides different deep learning architectures for CMF detection. Finally, conclusions and future research directions are explained in section V.

2. Block-Based Copy-Move Forgery Detection Methods

Block-based techniques segments input image into $(M- S+1)\times(N-S+1)$ overlapping blocks of equal size $S\times S$, where size of the image is $M\times N$. Vertical and horizontal direction sliding window overlapping blocks ensures presence of any duplicate regions. In the second stage, feature vector is extracted from each blocks using different techniques such as discrete wavelet transform (DWT), discrete cosine transform (DCT), singular value decomposition (SVD), logpolar transform, LBP and moments. Lastly, similar feature vectors are matched and localization of the doctored region is accomplished using various post processing and morphological operations. Lexicographic sorting is popular choice for sorting the feature vector. Fig. 3 depicts the generalized framework for block-based CMF detection algorithms.

DCT based color moments and combination of five image block features are employed to enhance robustness against post-processing operations like JPEG compression and blurring in [10]. Clustering based on similar color groups and overlapping blocks are obtained and color features are extracted from the input test image. Additionally, these features are trained using an deep compositional neural network ensemble model and forged regions are detected. After converting input RGB image into grayscale, it is divided into overlapping blocks and histogram of orientated Gabor magnitude (HOGM) descriptor is extracted [11]. Forged regions are detected using lexicographic sorting of feature vectors by identifying similarity in the block pairs. Robustness experiments against multiple CMF are also evaluated in the proposed approach. Feature extraction and matching based on fast Fourier transform (FFT), singular value decomposition (SVD), and principal component analysis (PCA) is utilized in [12]. Different block matching including city block, horizontal and vertical are applied to detect duplicated regions with localization. The proposed algorithm achieved detection rate of 98% and FNR of 6% at JPEG Q=20.

Combination of stationary wavelet transform (SWT) and DCT is developed using the approximation sub-band in [13]. The sub-band coefficients are segmented into overlapping

blocks and reduced feature vector is obtained using DCT for identifying similar forged areas. Non-subsampling or undecimated wavelet transform (UWT) and Zernike moments based copy-move forgery detection and localization technique is presented in [14]. Input is first decomposed into LL and HH sub-band using UWT and segmented into overlapping blocks and then similarity is obtained. Distance matrix for marching and manipulation detection is constructed using Zernike moments. Gaussian low-pass filter pre-processing on the input image is employed and divided into overlapping circular blocks in [15]. Quaternion exponent moments (QEMs) features are then extracted from each block and Euclidean hashing based block matching procedure is used for forgery detection.

In [16], image is first tranformed into overlapping blocks and blur moment invariants are illustrated for CMF. PCA and a k–d tree aids to analyze block similarity and to create duplicated segment map. After dividing an image into overlapping blocks, DCT transformation is carried out representing feature vector in [17]. The feature vector dimension is reduced by truncation and further lexicographic sorting and matching is performed in order to detect and localize forged region. The proposed approach demonstrated improved detection accuracy against JPEG compression, noise or blurring attack. The undecimated dyadic wavelet transform (DyWT) decomposition-based approximation and detail sub-bands are used for CMFD in [18]. The presented technique demonstrated EER =3.56 in case of JPEG compression with Q=90.

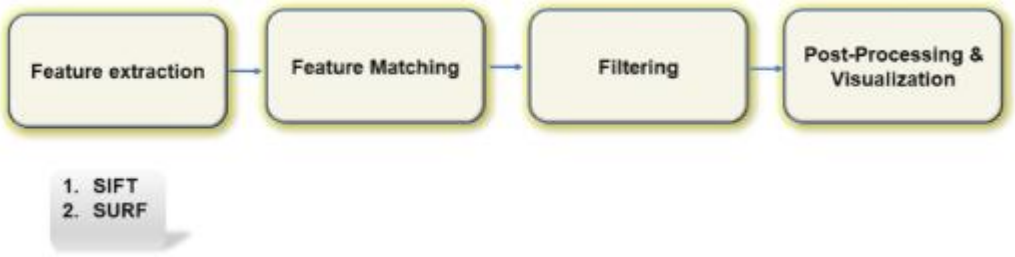

Figure 4: Key-point feature based matching steps for CMF detection

Block-based DCT feature extraction approach is explored which is robust against post-processing noise, blurring and compression attacks for CMF detection [19]. DCT feature vector is constructed using cellular automata and k-d tree nearestneighbor feature matching finally employed. The investigated techniques resulted in precision of 99.71% and F-score of 99.13%. From the circular overlapping blocks, polar complex exponential transform (PCET) features are extracted and SVD is used to reduce the dimensionality [20]. The implemented approach has low computational complexity and histogram similarity measure is utilized for block matching and the method is robust against rotation and scaling attacks. Firstly, the input image is decomposed using stationary wavelet transform (SWT) and low approximation sub-band ie extracted and DCT and SVD based feature selection is proposed for CMF detection in [21]. Only three features are used for matching the duplicated regions with accuracy of 99.61%. Moreover, the method

performs well against various attacks like, rotation, compression, scaling, and histogram equalization.

The method based on Polar Complex Exponential Transform (PCET) features and feature selection using Gradient Direction Pattern (GDP) histogram is investigated for CMF detection [22]. Feature matching and localization is obtained through histogram feature matching process with precision of 99.50%. Local tetra pattern (LTP) textural descriptor based features are extracted from overlapped blocks and lexicographically sorted for similar block matching in [23]. Experiments are conducted using two datasets: GRIP and CoMoFoD. Table I illustrates various block-based copy-move forgery detection algorithms.

3. Keypoint-Based Copy-Move Forgery Detection Algorithms

This approach provides feature key-point present within an image for similarity measurement. The scale-invariant feature transform (SIFT) [24] and Speeded-Up Robust Features (SURF) [25] are most popular methods for key-point feature extraction. Sometimes hybrid method which is the combination of both key-points (SURF and SIFT) are also exercised for forgery detection. Fig. 4 shows steps involved in algorithms developed for copy-move forgery detection using key-point feature marching.

As depicted in the fig. 4, SIFT or SURF key-point features are extracted and employed for detecting doctoring operation.

SIFT attains good detection rate in the presence of rotation and illumination modification attacks, whereas, SURF features extract local geometric image shift. Later, key-point feature matching and filtering process is applied to identify similarity. Finally, forged region identification and localization visualization will be presented by each matching key-point line transformation. As compared to block-based CMF, keypoint methods offers low computational cost and memory requirements.

The difficulty of large number and local spread of key-points is addressed by considering only strongest key-points chosen from Difference of Gaussian (DoG) and FAST-corner keypoints in [26]. Further, to reduce feature dimensions, DWT and football game based optimization (FGBO) algorithm is used. Experimental evaluations are performed using randomly collected 500 images from Internet resulting 96% of average accuracy. An improved CMF detection algorithm with reduced false matches using SIFT descriptors is proposed in [27]. The false matches are lowered by utilizing density clustering and outlier removal technique. The method demonstrated enhanced detection rate even in the presence of various attacks. The SIFT key-point descriptors are extracted first from the input image and robust features are identified and selected for feature matching [28]. Forged region localization is realized using Ciratefi approach and morphological operations. The proposed approach is robust against geometric distortion and degradation attacks.

Table 1: Block-Based Cmf Detection Algorithm Comparison

Algorithm	Year	Extracted Features	Classifier	Database	Performance Measures
[10]	2016	Color moments & Five block-based descriptors	CPNN	CoMoFoD	Accuracy & FNR
[11]	2015	HOGM	Euclidean distance	CoMoFoD & IMD	CDR & FDR
[12]	2017	FFT, SVD, PCA	Euclidean distance	CASIA v1.0	Accuracy & FNR
[13]	2018	SWT & DCT	Feature matching	CoMoFoD & UCID	TDR and FDR
[14]	2016	UWT & Zernike moments	Feature matching	CASIA v1.0	Accuracy, FPR, FNR
[15]	2018	QEM	E2LSH block matching	CoMoFoD	Precision, Recall, F-Score
[16]	2007	Blur moments	Similarity measure	Authors own database	Detection map
[17]	2011	DCT	Similarity matching	Columbia database	Accuracy, FPR and FNR
[18]	2012	DyWT	Distance measure	CASIA v1.0	Accuracy, FPR & FNR
[19]	2020	DCT	K-d tree	CoMoFoD	Precision, recall & F-score
[20]	2020	PCET-SVD	Histogram block measure	CoMoFoD & CASIA	Precision, recall & F-score
[21]	2023	SWT & SVD	Similarity matching	CoMoFoD	Accuracy & FPR
[22]	2023	PCET	Histogram features	CoMoFoD & CASIA	Recall, Precision, F-score
[23]	2023	LTP	Euclidean distance	GRIP & CoMoFoD	Pfrecision, Recall, F-score

The input image is first enhanced based on dynamic histogram equalization (DHE) and SURF descriptors are extracted for CMF detection [29]. Finally, binary mask is generated using modified density-based spatial clustering of application with and forged regions are located. 92.88% precision is achieved using the developed approach. An enhanced threshold based SURF key-point descriptors are proposed to detect CMF with detection accuracy of 97% [30]. Peroframnce evaluation is carried out on CASIA database. An accelerated KAZE features and Hamming distance matching is developed for copy-move detection in [31]. DBSCAN for key-point clustering is utilized and morphological processing is applied for tampered region localization.

The method illustrated identifies uniformly distributed image key-points for improved forgery detection rate using SURF descriptors [32]. Additionally, PCA dimension reduction technique is employed for optimal feature clustering and for reducing false matching. 320 medical images are used for evaluation and the algorithm demonstrated satisfactory performance in terms of sensitivity, precision and F-score. Two step matching procedure is developed for manipulation detection and localization in [33]. In the first step, local intensity order pattern (LIOP) keypoints are employed for finding approximate location, whereas, second step consists of iterative neighborhood addition comprising of entire forged region. Robust key-point pair matching and detection is performed by DBSCAN. The forgery detection technique based on SIFT key-point descriptors which is robust against translation, rotation, and scaling is presented in [34]. Besides, DBSCAN to cluster SIFT keypoints and similarity measure based on Hu's invariant moments are employed. Finally, region growing technique based forged area localization is implemented.

An adaptive scale-invariant feature transform (ADSIFT), gamma factor based feature matching and forgery detection using scaling factor is illustrated for CMF detection [35]. The proposed approach employs sufficient number of key-points that are collected from low-contrast or smooth area of input image to enhance detection performance. In [36], SURF keypoint descriptor based approach is developed for CM forgery detection and localization. Authors demonstrated robustness of the proposed approach against rescaling, blurring and rotation attacks. The key-point based techniques for CMF are tabulated in table II.

4. Deep Learning Based Techniques for Cmfd

Recently different researchers developed CMF detection algorithms using convolutional neural networks (CNN) [37]– [39]. The CNN architecture for splicing and copy-move forgery detection is illustrated in [40]. High-pass filter is employed to assign CNN first layer weights instead of random assignment. Then pre-trained model acting as a patch descriptor is used to extract dense feature set and fed to SVM classification algorithm. GoogleNet transfer learning model for multiple CMF is proposed to overcome the issue of generalization [41]. Additionally, fractional leader harris hawks optimization (FLHHO) based CNN weigh and bias optimization is demonstrated with average accuracy of 93% and TNR of 93.8%.

Table 2: Key-point based copy-move forgery detection algorithm comparison

Algorithm	Year	Method	Database	Performance measures
[26]	2020	SIFT & DoG	Internet	Precision, Recall, F-Score
[27]	2021	SIFT	MICC-F220 & IMD	TPR & FPR
[28]	2022	SIFT	GRIP & CMH	Accuracy, TPR & FPR
[29]	2021	SURF	CoMoFoD, MICC-F220 & MICC-F2000	Precision, Recall, F-Score
[30]	2021	SURF	CASIA	Accuracy, Precision, Recall
[31]	2021	AKAZE	IMD & MICC-F8	ROC
[32]	2021	SURF	Authors own database	Accuracy, Recall & F-score
[33]	2021	LIOP	MICC-F600 & IMD	Precision, Recall & F-score
[34]	2023	SIFT	CoMoFoD	Recall, FNR & F1-score
[35]	2023	ADSIFT	MICC-F220, MICC-F600, CMH + GRIPori & COVERAGE	TPR, FPR & F1-score
[36]	2023	SURF	CoMoFoD	TPR, FPR & F1-score

Input RGB image is first converted into YCbCr and DCT is applied over non-overlapping blocks of size $N \times N$ in [42]. The CNN model is supplied with DCT coefficients as features for forgery detection. The CNN architecture is trained and tested using CASIAv1 and CASIAv2 databases. Authors in [43] developed double dual CNN (D2CNN) for CMF detection each consisting of CNN models. The input test image is identified as original and forged using fully connected network and D2CN evaluated using MICC F-220 and MICC F-2000 datasets with accuracy of 98.48% and 97.83% respectively. Convolutional block attention module (CBAM) is proposed for feature extraction and forged area localization in [44]. The model combines spatial and channel attention descriptors that captures forgery information. CoMoFoD image database is utilized for experimental validation and performance verification using different post-processing operations. After contrast enhancement of input image based on wiener filtering-contrast limited enhanced histogram equalization (WE-CLAHE), feature extraction is performed using hybrid dual-tree complex wavelet trigonometric transform (Hybrid DTT) and VGGNet transfer learning model [45]. Improved horse herd optimization (IHH) for feature selection and adaptive density-based fuzzy clustering (ADFC) for forgery detection is presented with average accuracy of 99.23% on CASIA V1 and 98.75% on COVERAGE databases. A multiple asymmetric cross-layer connections and atrous spatial pyramid pooling (ASPP) based U-net model is developed for CMF detection [46]. The proposed model exploits multiple U-shaped modules with various depths which changes the receptive field capturing global and local details and in turn improving the localization accuracy of doctored area.

Conclusion

This article presents a brief survey of existing copymove forgery detection algorithms. CMF is most popular type of forgery and gained attention by researchers in last decade. This work covers traditional (block-based and keypoint based) methods and recently introduced deep learning model for CMF detection. The applicability and relevance of these categories are described with the help of generalized workflow. Moreover, major works in these categories along with their primary method utilized, database and performance measure is also listed. As observed, deep learning CMFD models outperforms conventional feature based algorithms in terms of detection accuracy. One major hindrance applying deep learning algorithms is limited availability of the CMFD datasets. Furthermore, the performance enhancement can be explored by machine learning and deep learning or transfer learning ensemble in future.

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THE M/G/1 RETRIAL QUEUE WITH BERNOULLI SCHEDULE

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Abstract
We consider an M/G/1 retrial queue with infinite waiting space, in which arriving customers who find the server busy join either (a) the retrial group with probability p in order to seek service again after a random amount of time, or (b) the infinite waiting space with probability $q(= 1-p)$, where they wait to be served. The joint generating function of the numbers of customers in the two groups is derived using the supplementary variable method. It is shown that our results are consistent with known results when $p = 0$ or $p = 1$.

Keywords: Retrial Queues, Supplementary Variable Method.

Introduction

Retrial queueing systems are characterized by the feature that arrivals who find the server busy join a retrial group and try again for service, in random order and at random intervals. Retrial queues have been widely used to model problems arising in telephone switching systems and in computer and communication systems. For a comprehensive survey of retrial queues, see Yang and Templeton [9]. Most papers on retrial queues have treated systems with no waiting position (see Alexandrov [1], Falin [3], Kulkarni [7, 8], Choo and Conolly [2], Greenberg [5], and Yang and Templeton [9]).

In this paper we consider a modified M/G/1 retrial queue with infinite waiting positions, in which arriving customers who find the server busy join either the retrial group with probability p, or the infinite waiting space (called the priority group) with probability q $(= 1 - p)$. A customer in the retrial group always attempts to obtain service directly and returns to the retrial group when the server is busy, so that he is served only when there are no customers in the priority group. This rule implies that customers in the priority group have non-preemptive priority over those in the retrial group.

In Section 2 we describe the model and use the supplementary variable method to derive the joint generating function of the numbers of customers in the two groups, together with the mean queue lengths. We show that our results are consistent with those already known in the literature when $p = 0$ or $p = 1$. In Section 3 we find the optimal value of p under a cost structure that assigns different costs per customer per unit time to the retrial and priority groups.

Related Bernoulli-schedule retrial models have since been developed in a number of directions, including general (non-exponential) retrial times [13, 11], batch arrivals [12], feedback and negative customers [14], working vacations [15], and heavy-tailed tail-asymptotic behaviour [16].

The Queue Length

We consider a single-server queueing system with infinite waiting space. Customers arrive according to a Poisson process with rate λ. An arriving customer obtains service immediately if the server is idle; otherwise he joins the retrial group with probability p, waiting a random amount of time before his next attempt, or the infinite waiting space (called the priority group) with probability $q = 1 - p$, where he waits to be served. Customers who are blocked on their first attempt are allowed to join the priority group, but a customer already in the retrial group has no option to join the priority group and always returns to the retrial group if he finds the server busy on a retrial attempt. A customer in the retrial group is served only when there are no customers in the priority group; thus customers in the priority group have non-preemptive priority over those in the retrial group.

The retrial time (the interval between two consecutive attempts made by a customer in the retrial group) is exponentially distributed with mean $1/\alpha$, and is independent of all previous retrial times and of all other random variables in the system. Service times are independent and identically distributed with p.d.f. $s(x)$ and mean b. Let

$$s^*(\theta) = \int_0^\infty e^{-\theta x} s(x)\, dx$$

be the Laplace transform of the service time S. It is easy to show that the system is stable provided $\rho = \lambda b < 1$. We consider only stable systems and investigate the queue-length distribution at an arbitrary time using the supplementary variable method.

At an arbitrary time, the state of the system can be characterized by the random variables $N_1, N_2, \tilde{S}$ and ξ, where N_1 is the number of customers in the priority group (excluding any customer in service); N_2 is the number of customers in the retrial group; $\tilde{S}$ is the remaining service time of the customer in service; and $\xi = 1$ if the server is busy and $\xi = 0$ otherwise. Denote the probabilities

$q_j = P(N_2 = j,\ \xi = 0), \qquad j = 0,1,2,\ldots;$

$p_{i,j}(x)dx = P(N_1 = i,\ N_2 = j,\ \tilde{S} \in (x, x + dx),\ \xi = 1), \qquad i,j = 0,1,2,\ldots;$

and their Laplace transforms

$$p^*_{i,j}(\theta) = \int_0^\infty e^{-\theta x} p_{i,j}(x)\, dx.$$

Note that $p^*_{i,j}(0) = P(N_1 = i, N_2 = j, \xi = 1)$ is the steady-state probability that there are i customers in the priority group, j customers in the retrial group, and the server is busy. The usual arguments lead to the differential-difference equations:

$$(\lambda + j\alpha)q_j = p_{0,j}(0), \qquad j \geq 0; \tag{1a}$$

$$-p'_{0,j}(x) = -\lambda p_{0,j}(x) + p\lambda p_{0,j-1}(x) + s(x)p_{1,j}(0) + (j+1)\alpha s(x)q_{j+1} + \lambda s(x)q_j, \quad j \geq 0; \tag{1b}$$

$$-p'_{i,j}(x) = -\lambda p_{i,j}(x) + p\lambda p_{i,j-1}(x) + q\lambda p_{i-1,j}(x) + s(x)p_{i+1,j}(0),\ i \geq 1,\ j \geq 0; \tag{1c}$$

where $p_{i,-1}(x) = 0$ for any x. Taking Laplace transforms of (1b) and (1c) gives

$$(\theta-\lambda)p^*_{0,j}(\theta)+p\lambda p^*_{0,j-1}(\theta)=p_{0,j}(0)-s^*(\theta)p_{1,j}(0)-(j+1)\alpha s^*(\theta)q_{j+1}-\lambda s^*(\theta)q_j, \quad (2b)$$

$$(\theta-\lambda)p^*_{i,j}(\theta)+p\lambda p^*_{i,j-1}(\theta)+q\lambda p^*_{i-1,j}(\theta)=p_{i,j}(0)-s^*(\theta)p_{i+1,j}(0). \quad (2c)$$

For complex z_2 with $|z_2| \le 1$, define the generating functions:

$$Q(z2)=\sum_{j=0}^{\infty} qjz2j, \quad Pi*(\theta,z2)=\sum_{j=0}^{\infty} p*i,j(\theta)z2j, \quad Pi(0,z2)=\sum_{j=0}^{\infty} pi,j(0)z2j.$$

From equations (1a), (2b) and (2c) we obtain

$$\lambda Q(z_2)+\alpha z_2 Q'(z_2)=P_0(0,z_2), \quad (3a)$$

$$(\theta-\lambda+p\lambda z_2)P_0^*(\theta,z_2)=P_0(0,z_2)-s^*(\theta)P_1(0,z_2)-\alpha s^*(\theta)Q'(z_2)-\lambda s^*(\theta)Q(z_2), \quad (3b)$$

$$(\theta-\lambda+p\lambda z_2)P_i^*(\theta,z_2)+q\lambda P_{i-1}^*(\theta,z_2)=P_i(0,z_2)-s^*(\theta)P_{i+1}(0,z_2). \quad (3c)$$

Next we introduce the generating functions of $P_i^*(\theta,z_2)$ and $P_i(0,z_2)$:

$$P^*(\theta,z_1,z_2)=\sum_{i=0}^{\infty} P_i^*(\theta,z_2)z_1^i, \quad P(0,z_1,z_2)=\sum_{i=0}^{\infty} P_i(0,z_2)z_1^i.$$

Note that $P^*(0,z_1,z_2)=E(z_1^{N_1}z_2^{N_2};\ \xi=1)$, which is the joint generating function of (N_1,N_2) when the server is busy. From (3b) and (3c) we obtain

$$(\theta-\lambda+p\lambda z_2+q\lambda z_1)P^*(\theta,z_1,z_2)=\left[1-\frac{s^*(\theta)}{z_1}\right]P(0,z_1,z_2)+\frac{s^*(\theta)}{z_1}P_0(0,z_2) - \alpha s^*(\theta)Q'(z_2)-\lambda s^*(\theta)Q(z_2). \quad (4)$$

Choosing $\theta=\lambda-p\lambda z_2-q\lambda z_1$, we eliminate $P^*(\theta,z_1,z_2)$ and obtain

$$[z_1-s^*(\lambda-p\lambda z_2-q\lambda z_1)]P(0,z_1,z_2)=-s^*(\lambda-p\lambda z_2-q\lambda z_1)P_0(0,z_2) + z_1 s^*(\lambda-p\lambda z_2-q\lambda z_1)\big(\alpha Q'(z_2)+\lambda Q(z_2)\big). \quad (5)$$

Now consider the function

$$f(z_1,z_2)=z_1-s^*(\lambda-p\lambda z_2-q\lambda z_1). \quad (6)$$

For each fixed z_2 with $|z_2|<1$, regard $f(z_1,z_2)$ as a function of z_1. On the unit circle $|z_1|=1$ we see that

$$\mathrm{Re}(\lambda-p\lambda z_2-q\lambda z_1)=\lambda\big(1-p\,\mathrm{Re}(z_2)-q\,\mathrm{Re}(z_1)\big)>0.$$

Since $|s^*(\theta)|<1$ for $\mathrm{Re}(\theta)>0$, we must have $|s^*(\lambda-p\lambda z_2-q\lambda z_1)|<|z_1|$ on $|z_1|=1$. By Rouché's theorem it follows that, for each z_2 with $|z_2|<1$, there is a unique solution $z_1=\varphi(z_2)$ of the equation $f(z_1,z_2)=0$ within the unit circle, i.e.

$f(\varphi(z_2),z_2)=\varphi(z_2)-s^*(\lambda-p\lambda z_2-q\lambda\varphi(z_2))=0$. On the other hand, since

$$\left.\frac{\partial f(z_1,z_2)}{\partial z_1}\right|_{z_1=1,\,z_2=1}=1-qp>0,$$

we conclude by the implicit function theorem that $z_1=\varphi(z_2)$ is analytic on $|z_2|<1$ and continuous at $z_2=1$, with $\varphi(1)=1$.

We need the first and second derivatives of $\varphi(z_2)$ at $z_2=1$. It is easily seen that

$$\varphi'(1) = \frac{p\rho}{1-q\rho}, \qquad \varphi''(1) = \frac{p^2\lambda^2 E(S^2)}{(1-q\rho)^3}. \tag{7}$$

Returning to equation (5) and inserting $z_1 = \varphi(z_2)$ gives

$$Q'(z_2) = \frac{\lambda}{\alpha} \cdot \frac{1-\varphi(z_2)}{\varphi(z_2)-z_2} Q(z_2),$$

$$Q(z_2) = c \exp\left\{-\frac{\lambda}{\alpha}\int_{z_2}^{1} \frac{1-\varphi(x)}{\varphi(x)-x}\,dx\right\} \tag{8}$$

$P_0(0,z_2) = \alpha\varphi(z_2)Q'(z_2) + \lambda\varphi(z_2)Q(z_2).$ (9)

By equating (3a) and (8), we obtain the differential equation

whose solution is

Next we find $P^*(0,z_1,z_2)$ and the constant c simultaneously. Substituting (9) into (8) yields

$$P_0(0,z_2) = \lambda\varphi(z_2)\frac{1-z_2}{\varphi(z_2)-z_2} Q(z_2). \tag{10}$$

Thus $Q(z_2)$ and $P_0(0,z_2)$ are known, and $P(0,z_1,z_2)$ follows from (5). Finally, letting $\theta = 0$ in (4) and substituting $Q(z_2)$, $P_0(0,z_2)$ and $P(0,z_1,z_2)$ into (4), we obtain, after some calculation,

$$P^*(0,z_1,z_2) = c\frac{s^*(\lambda - p\lambda z_2 - q\lambda z_1) - 1}{pz_2 + qz_1 - 1} \cdot \frac{z_1 - \varphi(z_2)}{z_1 - s^*(\lambda - p\lambda z_2 - q\lambda z_1)} \times \frac{1-z_2}{\varphi(z_2)-z_2} \exp\left\{-\frac{\lambda}{\alpha}\int_{z_2}^{1}\frac{1-\varphi(x)}{\varphi(x)-x}\,dx\right\}. \tag{11}$$

To show that $c = 1-\rho$, we find $P^*(0,1,1)$ by letting $z_2 \to 1$ and then $z_1 \to 1$ in (11). Using $\varphi(1) = 1$ and (7), L'Hospital's rule gives

$$P^*(0,1,1) = c\frac{\rho}{1-\rho}.$$

From the total-probability relation $1 = Q(1) + P^*(0,1,1)$, we obtain $c = 1-\rho$ as the probability that the server is idle, and $P^*(0,1,1) = \rho$ as the probability that the server is busy — both as expected.

Theorem 1. *The stationary distribution of* (N_1,N_2,ξ) *has the following generating functions:*

$$Q(z_2) = E(z_2^{N_2};\xi=0) = (1-\rho)\exp\left\{-\frac{\lambda}{\alpha}\int_{z_2}^{1}\frac{1-\varphi(x)}{\varphi(x)-x}\,dx\right\}, \tag{12}$$

$$P^*(0,z_1,z_2) = E(z_1^{N_1}z_2^{N_2};\xi=1) = (1-\rho)\frac{s^*(\lambda-p\lambda z_2-q\lambda z_1)-1}{pz_2+qz_1-1}\cdot\frac{z_1-\varphi(z_2)}{z_1-s^*(\lambda-p\lambda z_2-q\lambda z_1)}\cdot\frac{1-z_2}{\varphi(z_2)-z_2} \times \exp\left\{-\frac{\lambda}{\alpha}\int_{z_2}^{1}\frac{1-\varphi(x)}{\varphi(x)-x}\,dx\right\}. \tag{13}$$

From (12), (13) and (7), algebraic manipulation gives the following mean queue lengths:

$$E(N_2;\xi=0) = \frac{\lambda}{\alpha}\rho p, \tag{14a}$$

$$E(N_2;\xi=1)=\frac{p\lambda^2E(S^2)}{2(1-\rho)(1-q\rho)}+\frac{\lambda}{\alpha}\cdot\frac{p\rho^2}{1-\rho}, \tag{14b}$$

$$E(N_1;\xi=1)=\frac{q\lambda^2E(S^2)}{2(1-q\rho)}. \tag{15}$$

Corollary 1. *The mean queue lengths in the two groups are given by*

$$E(N_2)=\frac{p\lambda^2E(S^2)}{2(1-\rho)(1-q\rho)}+\frac{\lambda}{\alpha}\cdot\frac{p\rho}{1-\rho},\qquad E(N_1)=\frac{q\lambda^2E(S^2)}{2(1-q\rho)}. \tag{16}$$

Remarks

The Theorem and Corollary are consistent with known results when $p = 0$ or $p = 1$.

(a) When $p = 1$, our model becomes the M/G/1 retrial queue with no losses. In this case $\varphi(z_2) = s^*(\lambda - \lambda z_2)$ and $N_1 = 0$. Equations (12) and (13) reduce to

$$Q(z_2)=E(z_2^{N_2};\xi=0)=(1-\rho)\exp\left\{-\frac{\lambda}{\alpha}\int_{z_2}^{1}\frac{1-s^*(\lambda-\lambda x)}{s^*(\lambda-\lambda x)-x}\,dx\right\},$$

$$P^*(0,1,z_2)=E(z_2^{N_2};\xi=1)=(1-\rho)\,\frac{1-s^*(\lambda-\lambda z_2)}{s^*(\lambda-\lambda z_2)-z_2}\,Q(z_2),$$

which agree with Theorem 6 in Falin [3]. The generating function of the queue length in the system is $Q(z_2) + z_2P^*(0,1,z_2)$, which equals

$$\frac{(1-\rho)(1-z_2)s^*(\lambda-\lambda z_2)}{s^*(\lambda-\lambda z_2)-z_2}\exp\left\{-\frac{\lambda}{\alpha}\int_{z_2}^{1}\frac{1-s^*(\lambda-\lambda x)}{s^*(\lambda-\lambda x)-x}\,dx\right\},$$

in agreement with equation (3.11) in Yang and Templeton [9].

(b) When $p = 0$, our model becomes the ordinary M/G/1 queue, and $N_2 = 0$. Equations (12) and (13) reduce to

$$Q(1)=P(\xi=0)=1-\rho,\qquad P^*(0,z_1,1)=E(z_1^{N_1};\xi=1)=(1-\rho)\,\frac{s^*(\lambda-\lambda z_1)-1}{z_1-s^*(\lambda-\lambda z_1)}.$$

The generating function of the queue length in the system is $Q(1) + z_1P^*(0,z_1,1)$, which equals

$$\frac{(1-\rho)(1-z_1)s^*(\lambda-\lambda z_1)}{s^*(\lambda-\lambda z_1)-z_1},$$

the Pollaczek–Khinchine formula.

Optimal Values of *q*

Suppose it costs \$A and \$B per customer per unit time in the priority group and the retrial group, respectively. We want to find the optimal parameter q that minimizes the expected total cost per unit time. Using (16), the expected total cost can be expressed as

$$T(q)=A\,E(N_1)+B\,E(N_2)=\frac{\lambda^2E(S^2)}{2(1-q\rho)}\left[qA+\frac{1-q}{1-\rho}B\right]+\frac{\lambda}{\alpha}\cdot\frac{(1-q)\rho}{1-\rho}B. \tag{17}$$ This gives

$$T'(q)=\frac{\lambda^2E(S^2)}{2(1-q\rho)^2}(A-B)-\frac{\lambda}{\alpha}\cdot\frac{\rho}{1-\rho}B.$$

If

$$\frac{A}{B} > \frac{2\rho}{(1-\rho)\alpha\lambda E(S^2)} + 1, \tag{18}$$

then $T'(q) > 0$ for $0 < q < 1$, so $T(q)$ is increasing; hence $q^* = 0$ is optimal. If

$$\frac{A}{B} < \frac{2\rho(1-\rho)}{\alpha\lambda E(S^2)} + 1, \tag{19}$$

then $T'(q) < 0$ for $0 < q < 1$, so $T(q)$ is decreasing; hence $q^* = 1$ is optimal. If

$$\frac{2\rho(1-\rho)}{\alpha\lambda E(S^2)} + 1 < \frac{A}{B} < \frac{2\rho}{(1-\rho)\alpha\lambda E(S^2)} + 1, \tag{20}$$

then $T(q)$ is a convex function and its minimum occurs at $T'(q) = 0$, giving the optimal value

$$q^* = \frac{1 - \sqrt{\frac{1-\rho}{2\rho}\,\alpha\lambda E(S^2)\left(\frac{A}{B} - 1\right)}}{\rho}.$$

Remark

Recently the authors found that this model is essentially identical to the retrial model with two-way communication and an infinite source of outgoing calls investigated by Falin [4], who wrote down the joint generating function of $(N_1 + 1, N_2)$ without proof. In our model this can be obtained as $z_1 P^*(0, z_1, z_2) + Q(z_2)$. However, in [4] there is an error in the mean waiting time, which is easily checked by considering the special cases $\rho = 0$ or $r = 0$, where the waiting time of an arbitrary customer is measured from the epoch he enters the system until the epoch service begins.

To apply the conventional notion of waiting time as above, an arriving customer who obtains service immediately is regarded as a member of the retrial group and the priority group with probability p and q, respectively. Using Little's formula, $EN_2 = \lambda p W_2$, the mean waiting time for each group is obtained from (14) as

$$W_2 = \frac{1}{1-\rho}\left[\frac{\rho}{\alpha} + \frac{\lambda E(S^2)}{2(1-q\rho)}\right], \qquad W_1 = \frac{\lambda E(S^2)}{2(1-q\rho)}.$$

However, if W_2 is defined as the mean waiting time only for customers who must wait in the retrial group, then the formula $EN_2 = \lambda p \rho W_2$ should be used instead.

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NANOMATERIALS IN PIGMENT SCIENCE: PHYSICAL PRINCIPLES, SYNTHESIS, AND EMERGING APPLICATIONS

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Abstract

Colour has traditionally been engineered through the chemistry of molecular dyes and bulk inorganic pigments, but the last two decades have witnessed a paradigm shift toward nanoscale colorants whose optical response is governed as much by physics as by chemistry. This chapter examines the convergence of condensed-matter physics, materials science, and colour technology that has given rise to the field of nanomaterial-based pigments. The physical mechanisms responsible for colour generation at the nanoscale — quantum confinement, localized surface plasmon resonance, Mie and Rayleigh scattering, and photonic bandgap effects in periodic nanostructures — are discussed in relation to conventional charge-transfer and crystal-field colouration in bulk pigments. The major classes of nanopigments, including plasmonic metal nanoparticles, quantum dots, metal-oxide-based cool pigments, and structurally coloured photonic architectures, are reviewed along with representative synthesis routes and characterization strategies. Applications spanning energy-efficient coatings, smart textiles, anti-counterfeiting security inks, cosmetics, sensing platforms, and display technologies are surveyed, and the environmental and toxicological considerations that accompany the use of engineered nanoparticles in colour applications are critically discussed. The chapter concludes by identifying the scientific and technological challenges that must be addressed for nanopigments to transition from laboratory curiosities to sustainable, large-scale colorant technologies, illustrating how fundamental physics continues to bridge discovery and application in modern pigment science.

Keywords: Nanopigments, Structural Colour, Plasmonics, Quantum Dots, Photonic Crystals, Cool Pigments, Nanomaterials.

1. Introduction

Colour is one of the oldest and most universal interfaces between physics and human technology. From ochre pigments used in prehistoric cave art to the synthetic azo dyes of the industrial era, the ability to generate and control colour has always depended on manipulating how matter absorbs, scatters, and re-emits light. Conventional pigments derive their colour from electronic transitions in molecules or crystal fields in transition-metal compounds, processes that are well described by classical chemistry. Over the past two decades, however, the emergence of nanotechnology has introduced a fundamentally different route to colouration, one in which the

size, shape, and spatial arrangement of matter at the nanometre scale — rather than its chemical identity alone — determines the perceived colour.

When the physical dimensions of a material approach the wavelength of visible light (approximately 380–750 nm) or the de Broglie wavelength of charge carriers, quantum-mechanical and electromagnetic effects that are negligible in bulk matter become dominant. Semiconductor nanocrystals exhibit size-tunable band gaps due to quantum confinement; noble-metal nanoparticles display intense, tunable colours arising from the collective oscillation of conduction electrons; and periodic nanostructures generate vivid, non-fading structural colours through constructive interference rather than pigment-based absorption. These phenomena collectively define the emerging discipline of nanopigment science, a field that sits precisely at the convergence of physics, chemistry, and applied materials engineering.

This chapter is organized to reflect that convergence. Section 2 establishes the physical principles that govern colour generation at the nanoscale. Section 3 classifies the major families of nanomaterial-based pigments. Section 4 outlines representative synthesis strategies, and Section 5 summarizes characterization approaches used to correlate nanostructure with optical response. Section 6 surveys applications across coatings, textiles, cosmetics, sensing, and display technologies, while Section 7 addresses the environmental and toxicological dimensions of nanopigment deployment. The chapter closes with a discussion of open challenges and future directions in Section 8.

2. Physical Principles Governing Colour in Nanomaterials

2.1 Quantum Confinement and Band Gap Engineering

In bulk semiconductors, the energy gap between the valence and conduction bands is fixed by the material's crystal structure and chemical composition. When the physical size of a semiconductor crystal is reduced to a few nanometres — smaller than the exciton Bohr radius — the motion of charge carriers becomes spatially restricted, and the continuous energy bands of the bulk material collapse into discrete, size-dependent energy levels. This phenomenon, known as quantum confinement, allows the emission and absorption wavelength of a semiconductor nanocrystal (a quantum dot) to be tuned continuously across the visible spectrum simply by varying particle diameter, without any change in chemical composition. Cadmium selenide quantum dots, for example, can be tuned from blue-green to red emission as particle size increases from roughly 2 to 8 nm.

2.2 Localized Surface Plasmon Resonance

Noble-metal nanoparticles such as gold and silver owe their striking colours to localized surface plasmon resonance (LSPR), the collective, resonant oscillation of conduction-band electrons driven by an incident electromagnetic field. When the frequency of incident light matches the natural oscillation frequency of the electron cloud, strong absorption and scattering occur at a

characteristic wavelength that depends sensitively on particle size, shape, composition, and the dielectric environment. Spherical gold nanoparticles typically appear ruby-red in colloidal suspension due to LSPR absorption near 520 nm, while aggregation or elongation into nanorods shifts the resonance toward longer wavelengths, producing a visible colour change from red to blue. This sensitivity of LSPR to interparticle spacing is the physical basis of colorimetric nanosensors, in which analyte-induced aggregation of gold or silver nanoparticles produces an easily observed colour transition.

2.3 Structural Colour and Photonic Bandgap Effects

A third and physically distinct mechanism of nanoscale colouration is structural colour, in which periodic variations of refractive index at length scales comparable to the wavelength of light produce colour through interference, diffraction, or coherent (Bragg-type) scattering rather than through selective absorption. Structural colours are the mechanism behind the iridescence of butterfly wings, peacock feathers, and opal, and they are reproduced synthetically in photonic crystals — ordered arrays of dielectric nanoparticles or block-copolymer domains whose periodicity defines a photonic bandgap that reflects a narrow band of wavelengths. Because the colour originates from geometry rather than from a chromophore that can bleach or degrade, structurally coloured pigments are inherently resistant to photobleaching and chemical fading.

2.4 Mie and Rayleigh Scattering in Nanopigments

For dielectric nanoparticles such as titanium dioxide, zinc oxide, or copper(I) oxide, colour and opacity are strongly influenced by elastic light scattering, described by Rayleigh theory when the particle is much smaller than the wavelength of light and by the more general Mie theory as particle size approaches the wavelength. The scattering efficiency and its wavelength dependence are governed by particle size, shape, and the refractive-index contrast with the surrounding medium, which explains why nanocrystalline metal-oxide pigments can be engineered to strongly reflect near-infrared radiation while remaining visually similar in colour to their conventional counterparts — a property exploited in solar-reflective "cool pigment" coatings.

3. Classification of Nanomaterial-Based Pigments

3.1 Plasmonic Metal Nanoparticle Pigments

Gold, silver, and copper nanoparticles constitute the archetypal plasmonic nanopigments. Their LSPR-derived colours are highly tunable through control of particle shape (spheres, rods, triangles, stars) and are widely exploited in colorimetric sensing, where a target analyte induces aggregation or etching of the nanoparticle surface and produces a visually detectable colour shift (Sabela *et al.,* 2017). Beyond sensing, plasmonic nanoparticles are being explored as durable, high-chroma colorants for glass, ceramics, and security inks, reviving a colouration strategy first

exploited empirically in mediaeval stained glass, now understood and engineered through modern electrodynamics.

3.2 Quantum Dot Pigments

Semiconductor quantum dots, including cadmium chalcogenides and increasingly heavy-metal-free alternatives such as indium phosphide/zinc sulfide (InP/ZnS) and carbon-based quantum dots, provide narrow-linewidth, size-tunable emission that gives them exceptional colour purity relative to conventional organic dyes. Quantum dot pigments are used to enhance colour gamut and brightness in liquid-crystal and organic light-emitting-diode displays, in high-security anti-counterfeiting inks, and increasingly in paints and coatings valued for their resistance to photobleaching. Concerns over the toxicity of cadmium-based quantum dots have accelerated research into heavy-metal-free formulations and carbon or graphene quantum dots, which combine luminescence with comparatively low toxicity and additional functionality such as ultraviolet shielding.

3.3 Structural-Colour and Photonic Crystal Pigments

Photonic-crystal pigments are constructed from monodisperse colloidal nanoparticles — silica, polystyrene, or inorganic core-shell particles — that self-assemble into ordered, close-packed arrays exhibiting angle-dependent structural colour (Zhu *et al.,* 2023). Related architectures include chiral nematic cellulose nanocrystal films, which self-assemble into left-handed helicoidal structures that selectively reflect circularly polarized light, and one-dimensional block-copolymer photonic crystals capable of stimuli-responsive colour change in response to humidity, temperature, or mechanical strain (Park *et al.,* 2023). Because these systems generate colour geometrically, they are inherently non-fading, and their responsiveness to external stimuli is being exploited in sensors, smart windows, and rewritable colour displays. Nature's own structural colourants — as seen in beetle cuticles that reflect circularly polarized light through helicoidal chitin architectures — continue to inspire synthetic designs (Sharma *et al.,* 2009).

3.4 Metal Oxide Nanopigments and Cool Pigments

Nanocrystalline metal oxides — titanium dioxide, zinc oxide, zirconium oxide, and mixed transition-metal oxide spinels — are widely used as "cool pigments" engineered to reflect a large fraction of incident near-infrared solar radiation while retaining conventional visible colouration, thereby reducing the surface temperature of coated buildings, vehicles, and pavements and mitigating the urban heat-island effect (Mansour and Farha, 2025). Because near-infrared reflectance depends on crystallite size, dopant concentration, and particle morphology, nanoscale control over these parameters allows cool-pigment performance to be tuned independently of visible-light colour, as demonstrated for particle-size-optimized $(Fe,Cr)_2O_3$ black pigments and gallium-doped zinc oxide nanocrystals (Toy *et al.,* 2025).

3.5 Carbon-Based and Bio-Inspired Nanopigments

Carbon dots, graphene quantum dots, and cellulose-nanocrystal-based photonic pigments represent a growing category of nanopigments derived from earth-abundant or renewable precursors. These materials combine tunable optical properties with comparatively favourable environmental and toxicological profiles relative to heavy-metal-based analogues, positioning them as sustainable alternatives within the broader effort to replace toxic legacy pigments such as cadmium- and lead-based compounds with safer, nanostructure-derived colorants (Jansen and Letschert, 2000; Wendusu *et al.,* 2015).

4. Synthesis Strategies

4.1 Top-Down Approaches

Top-down methods fabricate nanoscale colour-generating structures by physically or chemically sculpting bulk material. Techniques such as nanoimprint lithography, electron-beam lithography, and reactive-ion etching are used to pattern photonic-crystal colour filters and pixels with precise, angle-dependent optical response, offering excellent reproducibility for display and anti-counterfeiting applications, though typically at higher cost and lower throughput than solution-based routes. Ball milling is similarly used to reduce bulk metal-oxide pigments to the nanocrystalline size regime required for enhanced near-infrared reflectance in cool-pigment coatings.

4.2 Bottom-Up Approaches

Bottom-up synthesis builds nanostructures from molecular or ionic precursors through nucleation and controlled growth, and it dominates the production of plasmonic nanoparticles, quantum dots, and self-assembled photonic crystals. Chemical reduction of metal salts (for example, citrate or borohydride reduction of gold or silver ions) yields plasmonic nanoparticles whose size and shape are controlled through reaction kinetics, capping-agent chemistry, and seed-mediated growth. Colloidal synthesis of semiconductor quantum dots typically employs high-temperature injection of organometallic precursors into a coordinating solvent, followed by shell growth to passivate surface defects and improve photoluminescence quantum yield. Photonic-crystal pigments are commonly produced through self-assembly of monodisperse colloidal spheres via evaporation-induced sedimentation, template-assisted assembly, or microfluidic droplet templating.

4.3 Green and Biogenic Synthesis

Growing concern over the environmental footprint of conventional wet-chemical synthesis has driven interest in green and biogenic routes, in which plant extracts, microorganisms, or biopolymers serve as reducing and stabilizing agents for metal and metal-oxide nanoparticles. Biogenic silver and gold nanoparticles synthesized using plant extracts have been demonstrated for colorimetric sensing applications with performance comparable to conventionally

synthesized nanoparticles, while offering reduced use of hazardous reagents and improved biocompatibility. Cellulose nanocrystals extracted from plant biomass similarly provide a renewable building block for structurally coloured photonic pigments, aligning nanopigment production with broader sustainability objectives.

5. Characterization Techniques

Correlating nanostructure with optical performance requires a combined structural and spectroscopic characterization strategy. X-ray diffraction (XRD) is used to confirm crystal phase and, through peak broadening, to estimate crystallite size in metal-oxide nanopigments. Electron microscopy techniques — field-emission scanning electron microscopy (FESEM) and transmission electron microscopy (TEM) — provide direct imaging of particle size, shape, and periodic ordering in photonic-crystal assemblies. UV-visible-near-infrared diffuse reflectance spectroscopy quantifies both the visible colour coordinates and the near-infrared reflectance that determines cool-pigment performance, while UV-visible extinction spectroscopy of colloidal suspensions is the standard tool for tracking LSPR peak position and aggregation state in plasmonic nanoparticles. Photoluminescence spectroscopy characterizes the emission wavelength and quantum yield of quantum dot pigments, and Fourier-transform infrared spectroscopy (FTIR) is routinely used to confirm surface functionalization and polymer-matrix compatibility in pigment-loaded coatings.

6. Applications

6.1 Energy-Efficient Coatings and Cool Pigments

Near-infrared-reflective nanopigments incorporated into architectural coatings, roofing membranes, and pavement sealants reduce surface heat build-up and associated cooling energy demand, offering a passive strategy for mitigating the urban heat-island effect in dense urban environments (Mansour and Farha, 2025). Alkyd- and acrylic-based coatings formulated with titanium dioxide, zinc oxide, or zirconium oxide nanoparticles have demonstrated substantially improved near-infrared reflectance relative to conventional pigment formulations while maintaining comparable visible appearance, gloss, and hiding power.

6.2 Smart Textiles and Anti-Counterfeiting Security Inks

Structural-colour pigments based on photonic crystals and chiral nematic cellulose nanocrystals are being integrated into textile coatings and security inks, where their angle-dependent iridescence and non-fading durability are difficult to replicate with conventional printing technologies, making them attractive for brand protection and currency security features. Stimuli-responsive photonic pigments that change colour in response to humidity, mechanical strain, or solvent exposure add a further layer of covert or overt authentication that is difficult to counterfeit.

6.3 Cosmetics and Personal Care

Nanostructured mica-titania and metal-oxide composite pigments are used in cosmetic formulations to achieve pearlescent, colour-shifting, and high-chroma effects that are not achievable with conventional organic dyes, while nanocrystalline zinc oxide and titanium dioxide additionally provide ultraviolet protection. The dual optical and photoprotective functionality of these nanopigments is a direct consequence of the same size-dependent scattering physics described in Section 2.4.

6.4 Colorimetric Sensors and Diagnostics

The sensitivity of LSPR to the local dielectric environment makes gold and silver nanoparticles the basis of a large class of colorimetric sensors capable of naked-eye detection of heavy-metal ions, biomolecules, and pathogens through analyte-induced nanoparticle aggregation or etching (Sabela *et al.,* 2017). Structural-colour photonic-crystal sensors similarly exploit lattice-spacing changes induced by humidity, pH, or molecular binding to produce a visually observable colour shift, offering low-cost, instrument-free sensing platforms for environmental and point-of-care diagnostic applications (Fan *et al.,* 2021).

6.5 Displays and Optoelectronics

Quantum-dot colour filters and photonic-crystal structural-colour pixels are increasingly used to enhance colour gamut, brightness, and energy efficiency in liquid-crystal and light-emitting-diode display technologies. Because photonic-crystal colour pixels rely on interference rather than absorptive filtering, they can, in principle, achieve higher optical efficiency and improved viewing-angle performance than conventional colour-filter arrays.

6.6 Cultural Heritage and Art Conservation

Non-destructive spectroscopic identification of pigments — including nanostructured and structurally coloured historical materials — supports the conservation and authentication of paintings and artefacts, while modern nanopigment chemistry, informed by historical formulations such as gold-nanoparticle-coloured mediaeval glass, continues to inform the design of stable, non-toxic replacement pigments for restoration work.

7. Environmental and Toxicological Considerations

The same nanoscale dimensions that confer novel optical properties on nanopigments also raise legitimate concerns regarding occupational exposure, environmental release, and ecotoxicity. Cadmium-based quantum dots can release toxic cadmium and selenide ions upon weathering under acidic or alkaline conditions, motivating the development of heavy-metal-free alternatives such as InP/ZnS and carbon-based quantum dots. Silver and zinc oxide nanoparticles have likewise been identified as posing potential hazards to workers handling nanostructured inks and pigments, prompting surface-functionalization strategies intended to reduce reactivity and improve biocompatibility. Broader ecotoxicological studies indicate that engineered

nanoparticles can exhibit toxicity profiles distinct from their bulk counterparts, with outcomes strongly dependent on particle size, surface charge, and coating chemistry, underscoring the need for continued life-cycle and exposure-risk assessment as nanopigment technologies scale toward commercial production.

8. Challenges and Future Directions

- Scalable, low-cost synthesis: many high-performance nanopigments, particularly monodisperse photonic-crystal building blocks and precisely shaped plasmonic nanoparticles, remain difficult to produce at the volume and cost required for mass-market coatings and textiles.
- Heavy-metal-free formulations: continued substitution of cadmium- and lead-based nanopigments with InP/ZnS, carbon-based, and metal-oxide alternatives is needed to reconcile optical performance with toxicological safety.
- Durability and matrix compatibility: ensuring long-term colour stability, mechanical robustness, and weather resistance of nanopigments once dispersed within paint, textile, or polymer matrices remains an active area of formulation science.
- Standardized nanosafety assessment: harmonized protocols for evaluating occupational exposure and environmental release across the nanopigment life cycle are still under development.
- Multifunctional integration: combining structural colour, near-infrared reflectance, ultraviolet protection, and stimulus responsiveness within a single nanopigment platform represents a promising but technically demanding direction for future research.

Conclusion

Nanomaterial-based pigments exemplify how fundamental advances in condensed-matter and optical physics can be translated into technologies with immediate, tangible application — precisely the convergence of discovery and application that motivates this volume. Quantum confinement, plasmon resonance, and photonic bandgap engineering, once the province of basic physical research, now underpin commercial and emerging technologies in energy-efficient coatings, anti-counterfeiting security, cosmetics, sensing, and next-generation displays. Realizing the full potential of this field will depend on continued interdisciplinary collaboration between physicists, materials chemists, and process engineers to address outstanding challenges in scalable synthesis, long-term stability, and environmental safety, ensuring that the next generation of pigments is not only optically superior but also sustainable.

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NONLINEAR ROLL MOTION ANALYSIS OF SHIPS USING THE DUFFING OSCILLATOR MODEL

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Abstract

This study investigates the nonlinear roll motion of a ship using the Duffing equation with linear damping and a cubic nonlinear restoring moment under harmonic wave excitation. The governing nonlinear differential equation is solved using the Taylor Series Method (TSM), which provides a semi-analytical approximation of the roll response. A fourth-order Taylor series solution is obtained for the prescribed initial conditions and system parameters. Based on the derived solution, the corresponding damping and restoring moments are evaluated analytically. The results demonstrate that the Taylor Series Method accurately captures the nonlinear roll dynamics while providing a simple and computationally efficient approach for analyzing nonlinear ship motion under periodic wave loading.

Keywords: Duffing Equation, Ship Roll Motion, Taylor Series Method, Nonlinear Restoring Moment, Damping Moment.

1. Introduction

Ship roll motion is one of the most significant dynamic responses affecting the safety, stability, and operational performance of marine vessels. Excessive rolling can reduce crew comfort, damage cargo, and, in severe conditions, lead to loss of stability or capsize. Therefore, accurate mathematical modeling and analysis of ship roll motion are essential for ship design, stability assessment, and control system development. Early studies modeled ship roll using linear differential equations, which are suitable for small roll angles but fail to capture the complex behavior observed under large-amplitude wave excitation (Nayfeh & Mook, 1979).

In practice, the restoring moment of a ship exhibits nonlinear characteristics due to the variation of the righting arm (GZ) with heel angle. To account for this behavior, the restoring moment is commonly approximated by a cubic polynomial, leading to the Duffing equation. The Duffing model effectively represents nonlinear stiffness, resonance, jump phenomena, and multiple equilibrium states that cannot be described by linear models (Thompson & Stewart, 2002). Consequently, the Duffing equation has become a widely accepted mathematical model for investigating nonlinear ship roll dynamics.

Several analytical and numerical methods have been developed to solve nonlinear differential equations, including the Adomian Decomposition Method, Homotopy Perturbation Method, Variational Iteration Method, Differential Transform Method, Runge–Kutta methods, and the Taylor Series Method (He, 1999; Adomian, 1994). Among these techniques, the Taylor Series Method (TSM) is particularly attractive because it generates approximate analytical solutions by expanding the unknown function into a power series and recursively determining the coefficients from the governing equation and initial conditions. The method is simple to implement, computationally efficient, and provides high accuracy over a finite interval.

In this work, the Taylor Series Method is employed to obtain a fourth-order approximate solution of the Duffing equation for ship roll motion. Using the derived solution, the corresponding damping and nonlinear restoring moments are evaluated analytically. The obtained results demonstrate the capability of the Taylor Series Method to accurately describe nonlinear ship roll behavior while providing an efficient alternative to purely numerical solution techniques.

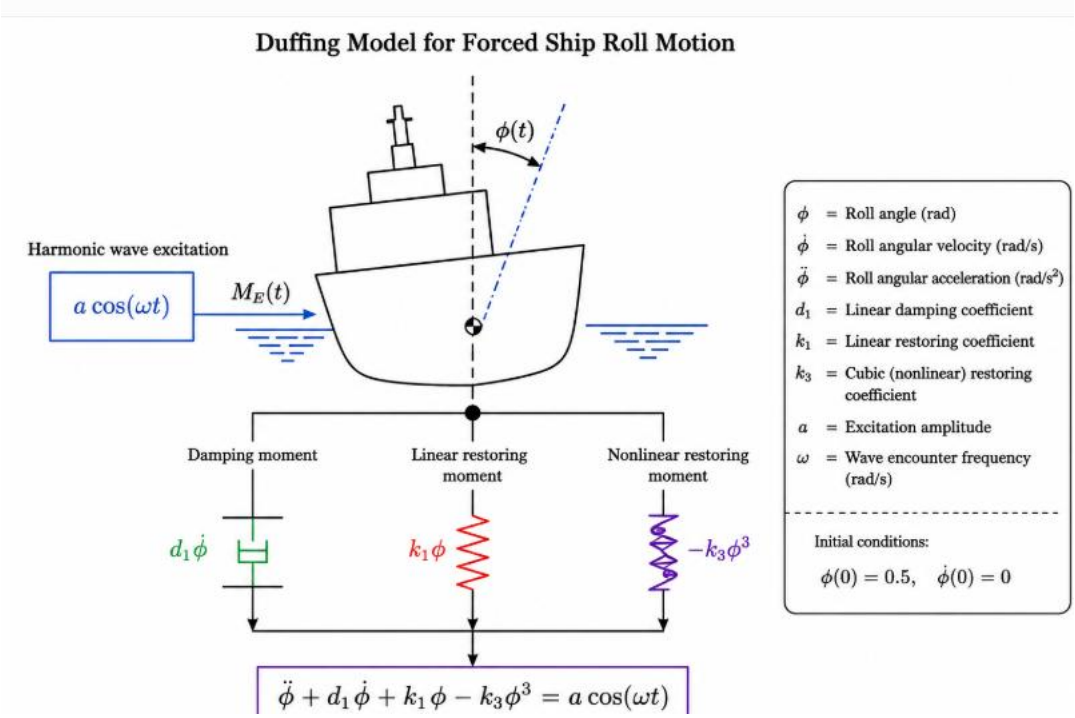


Figure 1: Schematic diagram for nonlinear roll motion of ship

2. Theory

The nonlinear Duffing equation for ship roll motion is

$$\ddot{\phi} + d_1\dot{\phi} + k_1\phi - k_3\phi^3 = a\cos(\omega t) \qquad (1)$$

subject to the initial conditions

$$\phi(0) = 0.5, \dot{\phi}(0) = 0 \qquad (2)$$

Where ϕ is the roll angle (rad), $\dot{\phi}(t)$is the roll angular velocity (rad/s), $\ddot{\phi}(t)$is the roll angular acceleration (rad/s^2), $d_1$is the linear damping coefficient, $k_1$is the linear restoring coefficient,

$k_3$is the cubic nonlinear restoring coefficient, $a$is the excitation amplitude, $\omega$is the excitation frequency (rad/s).

3. Result and Discussion

The Taylor Series Method (TSM) is a semi-analytical technique used to obtain approximate analytical solutions of nonlinear differential equations. It constructs the solution as a power series about the initial point, with the series coefficients determined recursively from the governing differential equation and the prescribed initial conditions. The method is particularly effective for nonlinear initial value problems because it provides highly accurate local approximations without requiring linearization or discretization.

Taylor Series Method assumes the solution in the form

$$\phi(t) = \sum_{n=0}^{\infty} \frac{\phi^{(n)}(0)}{n!} t^n, \tag{3}$$

$$\phi(t) = 0.5 + \frac{1}{2}\left(-\frac{k_1}{2} + \frac{k_3}{8} + a\right) t^2 - \frac{d_1}{6}\left(-\frac{k_1}{2} + \frac{k_3}{8} + a\right) t^3 + \frac{1}{24}\left[\left(d_1^2 - k_1 + \frac{3k_3}{4}\right)\left(-\frac{k_1}{2} + \frac{k_3}{8} + a\right) - a\omega^2\right] t^4 \tag{4}$$

Hence,

$$\phi(t) = 0.5 + 0.875625\, t^2 - 0.0291875\, t^3 - 0.0560147\, t^4 \tag{5}$$

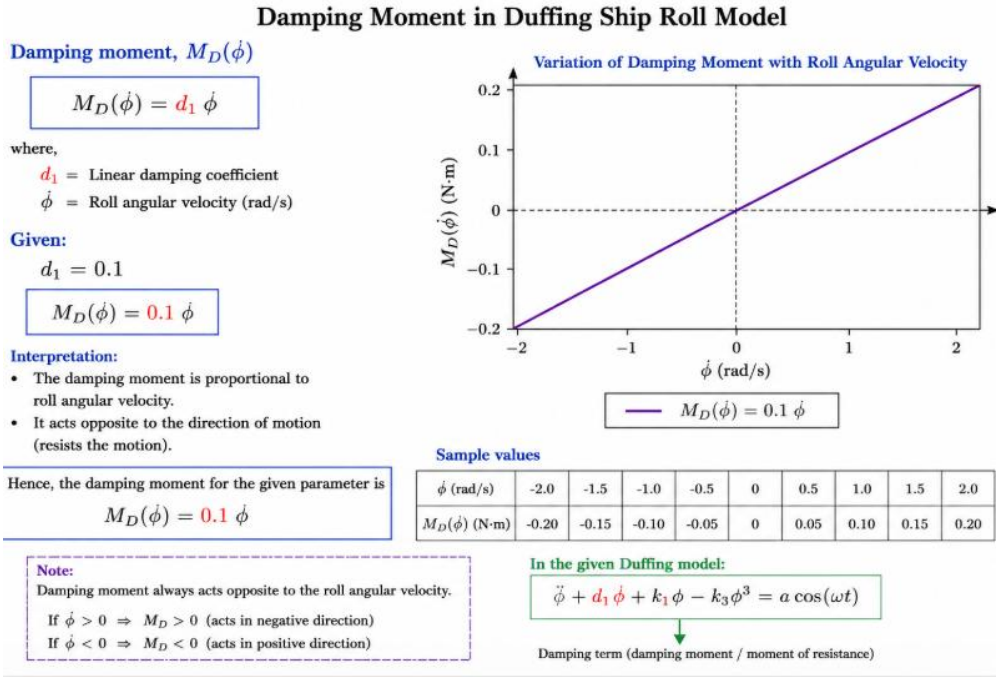
The experimental values of parameters

d_1=0.1, k_1=0.5, k_3 =0.01,a=2, ω=0.5 (6)

The damping moment is

$$M_D(\dot{\phi}) = d_1 \dot{\phi}, \tag{7}$$

$$M_D(t) = 0.175125\, t - 0.00875625\, t^2 - 0.02240588\, t^3 \tag{8}$$



The restoring moment is

$$M_R(\phi) = k_1\phi - k_3\phi^3, \tag{9}$$

Where

$$k_1 = 0.5,\ k_3 = 0.01.$$

Substituting

$$\phi(t) = 0.5 + 0.875625t^2 - 0.0291875t^3 - 0.0560147t^4$$

$$\phi^3(t) = 0.125 + 0.65671875\,t^2 - 0.021890625\,t^3 + 1.11722035\,t^4$$

Therefore,

$$M_R(t) = 0.5\phi - 0.01\phi^3$$
$$= 0.24875 + 0.43124531\,t^2 - 0.01437516\,t^3 - 0.03918555\,t^4. \tag{10}$$

Restoring Moment in Duffing Ship Roll Model

Restoring moment, $M_R(\phi)$

$$M_R(\phi) = k_1\phi - k_3\phi^3$$

where,

k_1 = Linear restoring coefficient

k_3 = Cubic (nonlinear) restoring coefficient

Given:

$k_1 = 0.5, \quad k_3 = 0.01$

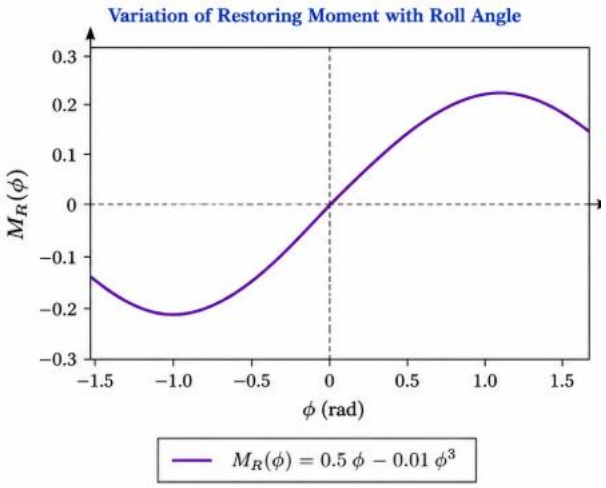
$$M_R(\phi) = 0.5\,\phi - 0.01\,\phi^3$$

Interpretation:

- For small angles, the term $k_1\phi$ dominates and the restoring moment is approximately linear.
- For large angles, the cubic term $-k_3\phi^3$ reduces the restoring moment (softening behavior).

Hence, the restoring moment for the given parameters is

$$M_R(\phi) = 0.5\,\phi - 0.01\,\phi^3$$



Sample values

ϕ (rad)	-1.5	-1.0	-0.5	0	0.5	1.0	1.5
$M_R(\phi)$	-0.2588	-0.2400	-0.1244	0	0.1244	0.2400	0.2588

Conclusion

This study presented the application of the Taylor Series Method (TSM) to obtain an approximate analytical solution of the nonlinear Duffing equation governing forced ship roll motion. The mathematical model incorporated linear damping, linear restoring stiffness, and a cubic nonlinear restoring moment under harmonic wave excitation. A fourth-order Taylor series solution was derived using the prescribed initial conditions and system parameters.

Based on the obtained roll response, analytical expressions for the damping moment and nonlinear restoring moment were evaluated. The results showed that the damping moment varies linearly with the roll angular velocity, while the restoring moment exhibits nonlinear softening behavior due to the cubic stiffness term. These characteristics enable the Duffing model to represent the nonlinear roll dynamics of a ship more realistically than the conventional linear model.

The study demonstrates that the Taylor Series Method is a simple, efficient, and accurate semi-analytical technique for solving nonlinear ship roll equations. The method provides reliable local approximations with relatively low computational effort and can be extended to higher-order expansions for improved accuracy. Therefore, it offers a useful alternative to purely numerical methods for analyzing nonlinear ship roll dynamics and can be applied to a wide range of engineering problems involving nonlinear oscillatory systems.

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RADIUS OF CONVEXNESS FOR CERTAIN CLASS OF UNIVALENT FUNCTIONS

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Abstract
In this paper, class of normalized univalent functions having fixed first t[th] coefficients is studied. Author overlook the geometric properties for this class. Also obtained the radius of convexness for the concern class.

Keywords. Normalized, Holomprphic, Convexness, Univalent.

1. Introduction

Let N be class of all holomprphic functions normalized with conditions:

$$\psi(z) = z + \sum_{k=2}^{\infty} a_k z^k, \qquad (1.1)$$

$\psi(0) = 0$ and $\phi'(0) = 1$

on open unit disc $\triangleright = \{z: |z| < 1\}$.

In this section we have defined new class of univalent functions with fixed first t[th] coefficients in unit disc$\triangleright$. Pawar [9] has studied the holomprphic functions having fixed second coefficient. Joshi [6] defined the class $S_{t,\beta}(\alpha, e, \gamma)$ of holomprphic functions. The class $S_{t,\beta}(\alpha, e, \gamma)$ consist of analytic functions ϕ in $\mathcal{HL}$

Satisfying:

$$\left| \frac{(\psi_{t,\beta}(z))' - 1}{e(\psi_{t,\beta}(z))' + 1 - (1+e)\gamma} \right| < \alpha, \qquad z \in \triangleright \qquad (1.2)$$

Where $(0 \leq e \leq 1, 0 < \alpha \leq 1, 0 \leq \gamma < 1)$ *and*

$$\psi_{t,\beta}(z) = z - \sum_{k=2}^{\infty} k^n C(\beta, k) l_k z^k, \quad C(\beta, k) = \prod_{i=2}^{k} (i - 2\ \beta) \quad \frac{\prod_{i=2}^{k} (i-2\ \beta)}{(k-1)!} \qquad (1.3)$$

Pawar [9] used this class to obtained new class $S_{t,\beta}(\alpha, e, \gamma, p)$ of holomprphic functions having fixed first second coefficient. Inspired with this [5] developed new class $\lambda - S^*_{\tau,t}(\partial, \sigma, p)$ of univalent functions having fixed first t[th] coefficients. For this, he studied geometric properties of the class $\lambda - S^*_{\tau,t}(\partial, \sigma)$ described by Ashwah [3] in details.

In [3] Ashwah used Salagean derivative operator to obtain the class $\lambda - S^*_{\tau,t}(\partial, \sigma)$ of univalent functions:

Definition 1.1 A function $\psi \in S$ is said to be in class $\lambda - S^*_{\tau,t}(\partial, \sigma)$ if

$$\mathrm{Re}\left\{\left(1 + \lambda e^{i\theta}\right) \frac{(1-\sigma)D^{\tau+1}\phi(z) + \sigma D^{\tau+2}\phi(z)}{(1-\sigma)D^{\tau}\phi(z) + \sigma D^{\tau+1}\phi(z)} - \lambda e^{i\theta}\right\} < \partial \qquad (1.4)$$

Where $1<\partial<\frac{4+\lambda}{3}$, $0\leq \sigma \leq 1$,$\theta \in \mathbb{R}$, $0 \leq \lambda<\infty$ and D^{τ} is Salagean derivative operator [9].

The expression for Salagean derivative operator is as follows:

$D^{\tau}\psi(z)= z+\sum_{k=2}^{\infty} k^{\tau} l_k z^k$,

We used following theorem to established our main results.

Theorem 1.1. Let $\psi(z) = z+\sum_{k=2}^{\infty} l_k z^k$, belongs to the class $\lambda - S^*_{\tau,t}(\partial,\sigma)$ iff

$$\sum_{k=2}^{\infty} k^{\tau}[1+\sigma(k-1)][k(1+\lambda)-\lambda-\partial]|l_k| \leq (\partial-1) \qquad (1.5)$$

Where $1<\partial<\frac{4+\lambda}{3}$, $0\leq \sigma \leq 1$,$\theta \in \mathbb{R}$, $0 \leq \lambda<\infty$

In concern with equation (1.5), the coefficients of the functions in the class $\lambda - S^*_{\tau,t}(\partial,\sigma)$ satisfy the bound

$$|l_k| \leq \frac{\partial-1}{k^{\tau}[1+\sigma(k-1)][k(1+\lambda)-\lambda-\partial]}, \qquad k \geq 2 \qquad (1.6)$$

Definition 1.2 [2] Convex functions

The function ψ is said to be convex, if it maps unit disc conformaly onto convex domain. The class of all convex function is denoted by Co. The class of all convex function is denoted by Co (α) for 0≤ α <1. If α=0, we get the class of convex function. Analytically convex function of order α is give as

$$\psi \in \text{Co}\ (\alpha) \Leftrightarrow \quad \text{Re}\{1+z\frac{\psi''(z)}{\psi'(z)}\}> t \qquad (1.7)$$

[5] introduced new class class $\lambda - S^*_{\tau,t}(\partial,\sigma,p)$ of normalized univalent functions having fixed first t^{th} coefficients. Different geometric properties studied for this class are growth theorem, convexness theorem, and extreme point theorem. [5] also obtained the radius of starlikeness for the class $\lambda - S^*_{\tau,t}(\partial,\sigma,p)$.

In this work, the class $\lambda - S^*_{\tau,t}(\partial,\sigma,p)$ *is studied* in more detail.

2. Main Result

Definition 2.1 Radius of convexness

Radius of **convexness** is maximum value of ρ ($\rho < 1$) such that functions $\psi(z)$ in N maps the image domain ($|z| < \rho$) onto convex domain.

In next theorem radius of convexness is obtained for this class $\lambda - S^*_{\tau,t}(\partial,\sigma,p)$

Theorem 2.1 Let the ψ be the function given by (4.8). If ψ is in $\lambda - S^*_{\tau,t}(\partial,\sigma,p)$, then ψ is convex of order ξ for the$|z|< \rho_1(\tau,t,\partial,\sigma,p)$.Where$\rho_1(\tau,t,\partial,\sigma,p)$ is maximum value which satisfies:

$$\sum_{h=2}^{t+1} \frac{hp(\partial-1)(h-\xi)}{h^{\tau}[1+\sigma(h-1)][h(1+\lambda)-\lambda-\partial]}\rho^{h-1} + \frac{k(1-tp)(\partial-1)(k-\xi)}{k^{\tau}[1+\sigma(k-1)][k(1+\lambda)-\lambda-\partial]}\rho^{k-1} \leq 1-\xi \qquad (2.1)$$

Where $k \geq t+1$, $0\leq \xi < 1$.

Proof: To obtain the result it is enough to show that

$$\left|\frac{z\psi''(z)}{\psi'(z)}\right| \leq 1 - \xi \qquad |z|<\rho_2$$

For $|z|<\rho_2 < 1$

$$\left|\frac{z\psi''(z)}{\psi'(z)}\right| = \left|\frac{\sum_{h=2}^{t+1} \frac{hp(\partial-1)(h-\xi)}{h^{\tau}[1+\sigma(h-1)][h(1+\lambda)-\lambda-\partial]}\, z^{h-1} + \sum_{k=t+2}^{\infty} k(k-1)l_k\, z^{k-1}}{1+\sum_{h=2}^{t+1} \frac{hp(\partial-1)}{h^{\tau}[1+\sigma(h-1)][h(1+\lambda)-\lambda-\partial]}\, z^{h-1} + \sum_{k=t+2}^{\infty} kl_k\, z^{k-1}}\right|$$

$$\leq \frac{\sum_{h=2}^{t+1} \frac{hp(\partial-1)(h-\xi)}{h^{\tau}[1+\sigma(h-1)][h(1+\lambda)-\lambda-\partial]}\, \rho^{h-1} + \sum_{k=t+2}^{\infty} k(k-1)|l_k|\, \rho^{k-1}}{1-\sum_{h=2}^{t+1} \frac{p(\partial-1)}{h^{\tau}[1+\sigma(h-1)][h(1+\lambda)-\lambda-\partial]}\rho^{h-1} - \sum_{k=t+2}^{\infty} k|l_k|\, \rho^{k-1}}$$

$$\leq 1 - \xi$$

Therefore,

$$\sum_{h=2}^{t+1} \frac{hp(\partial-1)(h-1)}{h^{\tau}[1+\sigma(h-1)][h(1+\lambda)-\lambda-\partial]}\, \rho^{h-1} + \sum_{k=t+2}^{\infty} k(k-1)|l_k|\, \rho^{k-1}$$

$$\leq (1-\xi)\left(1 - \sum_{h=2}^{t+1} \frac{hp(\partial-1)}{h^{\tau}[1+\sigma(h-1)][h(1+\lambda)-\lambda-\partial]}\rho^{h-1} - \sum_{k=t+2}^{\infty} k|l_k|\, \rho^{k-1}\right)$$

$$\Rightarrow \left(\sum_{h=2}^{t+1} \frac{ph(\partial-1)(h-\xi)}{h^{\tau}[1+\sigma(h-1)][h(1+\lambda)-\lambda-\partial]}\, \rho^{h-1} + \sum_{k=t+2}^{\infty} k(k-\xi)|l_k|\, \rho^{k-1}\right)$$

$$\leq (1-\xi)$$

Now given that

$\psi \in \lambda - S^*_{\tau,t}(\partial, \sigma, p)$,

$$|l_k| = \frac{(1-tp)(\partial-1)}{k^{\tau}[1+\sigma(k-1)][k(1+\lambda)-\lambda-\partial]}\, e_k$$

Where, $\sum_{k=t+2}^{\infty} e_k \leq 1$, $e_k \geq 0$. For fixed ρ select k_0= k (ρ) such that

$$\frac{k(k-\xi)}{k^{\tau}[1+\sigma(k-1)][k(1+\lambda)-\lambda-\partial]}\, \rho^{k-1}$$

is maximum.

$$\sum_{k=t+2}^{\infty} k(k-\xi)|l_k|\, \rho^{k-1} = \sum_{k=t+2}^{\infty} \frac{k(k-\xi)(1-tp)(\partial-1)e_k}{k^{\tau}[1+\sigma(k-1)][k(1+\lambda)-\lambda-\partial]}\, \rho^{k-1}$$

$$\leq \frac{k_0(k_0-\xi)(1-tp)(\partial-1)}{{k_0}^{\tau}[1+\sigma(k_0-1)][k_0(1+\lambda)-\lambda-\partial]}\, \rho^{k_0-1}$$

$$\Rightarrow \left(\sum_{h=2}^{t+1} \frac{ph(\partial-1)(h-\xi)}{h^{\tau}[1+\sigma(h-1)][h(1+\lambda)-\lambda-\partial]}\, \rho^{h-1} + \sum_{k=t+2}^{\infty} k(k-\xi)|l_k|\, \rho^{k-1}\right)$$

$$\leq \left(\sum_{h=2}^{t+1} \frac{ph(\partial-1)(h-\xi)}{h^{\tau}[1+\sigma(h-1)][h(1+\lambda)-\lambda-\partial]}\, \rho^{h-1} + \frac{k_0(k_0-\xi)(1-tp)(\partial-1)}{{k_0}^{\tau}[1+\sigma(k_0-1)][k_0(1+\lambda)-\lambda-\partial]}\, \rho^{k_0-1}\right)$$

$$\leq (1-\xi)$$

Then the radius of convexness is value ρ_0 such that:

$$\left(\sum_{h=2}^{t+1} \frac{ph(\partial-1)(h-\xi)}{h^{\tau}[1+\sigma(h-1)][h(1+\lambda)-\lambda-\partial]}\, {\rho_0}^{h-1} + \frac{k_0(k_0-\xi)(1-tp)(\partial-1)}{{k_0}^{\tau}[1+\sigma(k_0-1)][k_0(1+\lambda)-\lambda-\partial]}\, {\rho_0}^{k_0-1}\right) = (1-\xi)$$

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SPINEL FERRITE NANOMATERIALS: SYNTHESIS STRATEGIES, STRUCTURAL INSIGHTS, AND EMERGING TECHNOLOGICAL APPLICATIONS

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Abstract

Ferrites are highly studied inorganic nanomaterials because of their remarkable structural, optical, electrical, and magnetic properties. These versatile properties are responsible for their large-scale technological applications. Among the ferrite family, Spinels has attracted considerable attention because of high specific surface area, favourable magnetic, electric properties, good chemical stability along with relatively low resistivity compared with many other ferrites. Mixed metal ferrites find applications in photocatalysis, energy storage devices, gas sensing, water splitting, organic conversion etc. Ferrites are been synthesized by Sol-gel Autocumbustion method, Hydrothermal, Sonication Co-precipitation method etc.

Keywords: Ferrites, Normal Spinel, Inverse Spinel.

Introduction

Nanomaterials are very interesting particles (crystalline or amorphous) may be of organic or may be of inorganic materials possessing the sizes in the range of 1-100 nm. The unique properties of nanomaterials distinguish them from bulk.

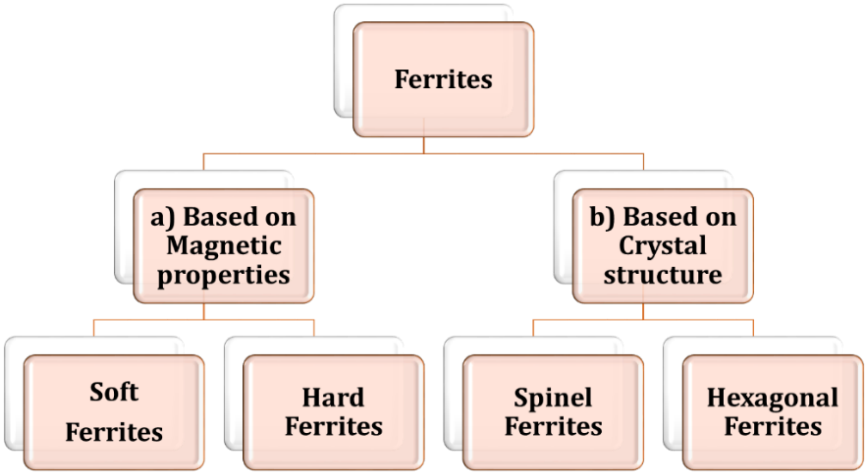

Figure 1: Classification of ferrites

These unique properties of nanomaterials are due to very small grain sizes; there is very huge percentage of the atoms situated in the grain boundary. Spinels are AB_2O_4 type of compounds

where, A is bivalent metal cation (Zn^{2+}, Cd^{2+}, Ni^{2+}) and B trivalent metal cation respectively, if the trivalent cation is iron, then they are termed ferrites [1]. Ferrites are classified based on crystal structure and magnetic properties.

Ferrites are further categorized into three kinds based on their crystal structure: i) Spinel ferrites ii) Hexagonal ferrites. In this chapter we are mainly focussing on Spinel ferrites. Spinel ferrites are further classified in three classes according to their distribution of cations over tetrahedral A site and octahedral B sites as (a) normal spinel, (b) inverse spinel and (c) mixed spinel.

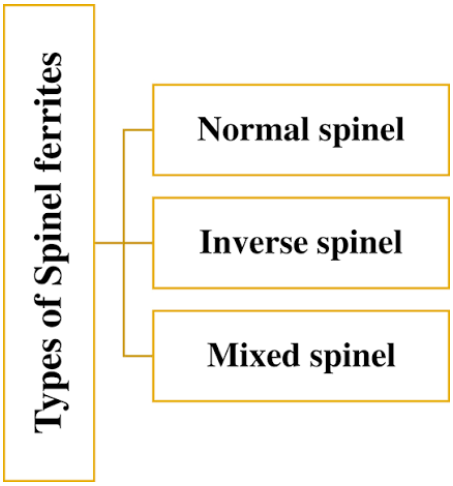

Figure 2: Classification of Spinel Ferrites [2]

a) Normal Spinel: The spinel is said to be a normal spinel if the tetrahedral A site is occupied by divalent cations (M^{2+}) and octahedral B site is occupied by trivalent cation(M^{3+}). [3]

b) Inverse Spinel: M^{3+} ions occupy both A and B sites in inverse spinel ferrite, and M^{2+} ions occupy B sites. (M^{3+}) $A[M^{2+}M^{3+}]BO_4$ is the formula for inverse spinel ferrites [4]

c) Mixed Spinel: In these kinds of spinel ferrites the cations are dispersed as a combination of normal and inverse spinel and thus they are represented as $(M_{1-\square}{}^{2+}\ M^{3+})\ A\ [M^{2+}M_{2-\square}{}^{3+}]BO_4$. [5]

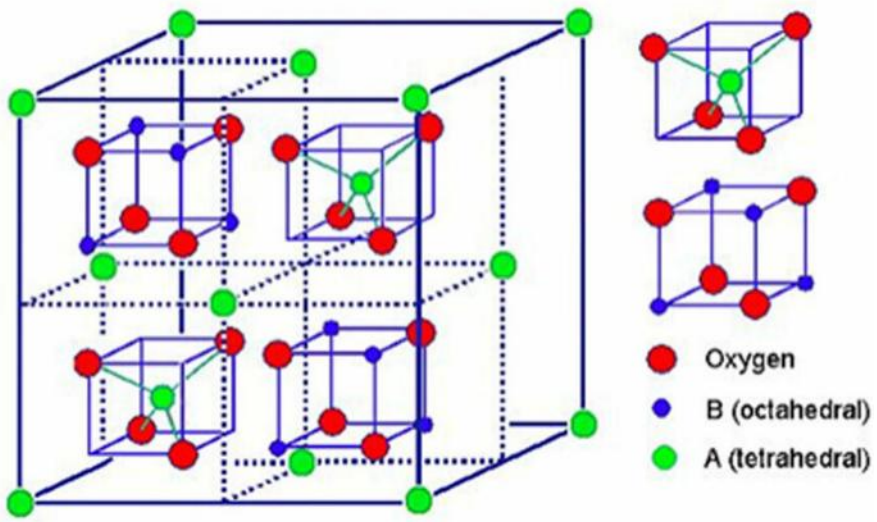

Figure 3: Structure of ferrite [6]

Ferrites are been synthesized by Sol-gel Autocumbustion method, Hydrothermal, Sonication Co-precipitation method etc. Literature studies have revealed that doping ferrites with different metals enhances structural, optical, magnetic and catalytic properties of ferrites [7-9]. Mixed metal ferrites find applications in photocatalysis, energy storage devices, gas sensing, water splitting, organic conversion etc. Agale *et al.* synthesized $Cu_{1-x}Ni_xMn_{1.0}Fe_2O_4$ by sol-gel auto-combustion method [10]. They had observed due to doping with Ni, electrochemical properties were enhanced in supercapacitors applications. *Vaibhav Salve et al.* synthesized $Zn_{1-x}Co_xMn_{1-x}FexCrO_4$ for high-performance supercapacitor applications [11]. The band gap of ferrite can be tuned by doping of metals for photocatalysis. *Santosh et al.* prepared $Cu_{0.5}Ni_{0.5}Mn_xFe_{2-x}O_4$ magnetically separable nano ferrites which was used as highly efficient photocatalyst for degradation of dye under solar light irradiation [12]. *Ishita et al.* synthesized $MgFeCrO_4$ NPs by aqueous combustion synthesis (ACS) using glycine as the fuel. Pyrano[2,3-c] pyrazole derivatives were synthesized in water/ethanol solvent system using $MgFeCrO_4$ NPs heterogenous catalyst [13]. Magnetic properties can also be enhanced by doping ferrites with different metals. There is drastic enhancement in the properties of $ZnFe_2O_4$ upon doping with suitable metal ions. The nonmagnetic Mg ions doped in $ZnFe_2O_4$ results in soft ferrite material which finds application for coil core. Literature studies revealed that even the non-magnetic divalent ions like $Zn^{2+}$and Mg^{2+} influence structural and magnetic properties of ferrites appreciably as they have different choices on the lattice sites. Ferrites has opened up several doors for future research into developing materials that are suitable for other applications such as hydrogen production, CO_2 reduction, solar cells, gas sensing, lithium-ion batteries etc.

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COPPER SULFIDE THIN FILMS: FUNDAMENTALS, SYNTHESIS, AND FUNCTIONAL APPLICATIONS

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1. Introduction

Copper sulfide (CuS) is one of the most extensively studied transition metal chalcogenides owing to its remarkable optical, electrical, thermal, and electrochemical properties. It belongs to the family of I–VI semiconductor compounds and has gained considerable attention as a promising material for optoelectronic, photovoltaic, sensing, photocatalytic, and energy-storage applications. The increasing demand for low-cost, environmentally friendly, and high-performance semiconductor materials has stimulated intensive research on CuS thin films over the past few decades. Compared with conventional semiconductors such as silicon and gallium arsenide, CuS offers several advantages, including earth abundance, relatively low toxicity, simple synthesis, high optical absorption coefficient, and compatibility with various low-temperature deposition techniques [1-3].

CuS exists in several stable and metastable phases depending on the copper-to-sulfur ratio. These include chalcocite (Cu_2S), djurleite ($Cu_{1.97}S$), digenite ($Cu_{1.8}S$), anilite (Cu_7S_4), geerite (Cu_8S_5), spionkopite ($Cu_{39}S_{28}$), and covellite (CuS). Among these phases, covellite CuS has attracted particular interest because of its unique hexagonal crystal structure, high electrical conductivity, strong visible-light absorption, and excellent chemical stability. The presence of copper vacancies and mixed-valence copper ions contributes significantly to its electrical transport behavior and enhances its suitability for photoelectrochemical and photovoltaic applications. The development of thin-film technology has greatly expanded the practical utility of CuS. Thin films require considerably less material than bulk counterparts while providing improved control over thickness, morphology, crystallinity, and surface properties. The high surface-area-to-volume ratio of thin films also facilitates efficient charge transfer and increases the number of active sites available for electrochemical and catalytic reactions. Consequently, CuS thin films have become attractive candidates for solar energy conversion, photodetectors, gas sensors, transparent electrodes, supercapacitors, lithium-ion batteries, sodium-ion batteries, hydrogen evolution catalysts, and flexible electronic devices [4-7].

The physical properties of CuS thin films depend strongly on the deposition technique and experimental parameters. Variables such as precursor concentration, complexing agent, solution

pH, deposition temperature, deposition duration, substrate type, and post-deposition annealing significantly influence the nucleation process, crystal growth, grain size, stoichiometry, and defect concentration. Careful optimization of these parameters enables the fabrication of high-quality films with tailored structural, optical, and electrical properties. Numerous deposition techniques have been employed for the preparation of CuS thin films. These include chemical bath deposition (CBD), successive ionic layer adsorption and reaction (SILAR), electrodeposition, spray pyrolysis, thermal evaporation, radio-frequency magnetron sputtering, pulsed laser deposition, chemical vapor deposition, atomic layer deposition, molecular beam epitaxy, and hydrothermal or solvothermal methods. Among these techniques, chemical bath deposition has emerged as one of the most attractive because of its simplicity, low equipment cost, low processing temperature, and suitability for depositing uniform films on substrates with complex geometries. Moreover, CBD enables large-area coating with good thickness control and is readily scalable for industrial production [8-11].

Recent advances in nanotechnology have significantly improved the performance of CuS thin films by controlling their morphology at the nanoscale. Nanostructured CuS films with flower-like, plate-like, spherical, porous, and hierarchical architectures exhibit enhanced surface area and improved charge transport, making them particularly attractive for photocatalysis, energy storage, and sensing applications. Furthermore, the incorporation of CuS into heterostructures with materials such as ZnO, TiO_2, CdS, MoS_2, graphene, reduced graphene oxide, and graphitic carbon nitride has resulted in enhanced light harvesting, efficient charge separation, and improved device performance. In addition to renewable energy applications, CuS has attracted attention in plasmonics because of its localized surface plasmon resonance (LSPR) in the near-infrared region. This property enables applications in photothermal conversion, infrared shielding, biomedical imaging, and optical switching. The combination of semiconducting behavior and plasmonic response distinguish CuS from many conventional semiconductor materials and broadens its technological significance.

Despite remarkable progress, several scientific and technological challenges remain. Precise control over phase composition, stoichiometry, crystal defects, and film adhesion is essential for achieving reproducible performance. Environmental stability under prolonged illumination, oxidation resistance, and interface engineering are also important considerations for practical device fabrication. Advances in precursor chemistry, defect engineering, nanostructure design, and scalable deposition techniques are expected to overcome these limitations and facilitate the commercialization of CuS-based technologies.

This chapter provides a comprehensive overview of CuS thin films, covering their crystal structure, CBD method, characterization techniques, physical properties, and its applications.

2. Crystal Structure and Fundamental Properties

Copper sulfide belongs to the family of copper chalcogenide compounds that exhibit a rich variety of crystal structures arising from different copper-to-sulfur ratios. The Cu–S binary system contains several stable and metastable phases, each possessing distinct structural, electronic, and optical characteristics. Among these, covellite (CuS) is the most extensively investigated phase because of its superior electrical conductivity, excellent optical absorption, and outstanding electrochemical activity. The crystal structure of CuS was first identified as a hexagonal lattice belonging to the $P6_3/mmc$ space group. Unlike many conventional semiconductors, CuS exhibits a layered crystal structure consisting of alternating copper and sulfur atomic planes. Sulfur atoms occupy two crystallographically distinct positions, while copper atoms are distributed in both trigonal planar and tetrahedral coordination environments. This unique arrangement results in anisotropic electrical transport and facilitates rapid charge-carrier movement along specific crystallographic directions.

The unit cell of covellite contains six atoms arranged in a compact layered framework. Typical lattice parameters reported for well-crystallized CuS are $a \approx 3.79$ Å and $c \approx 16.34$ Å, although slight variations occur depending on synthesis conditions, crystallinity, and residual strain within the thin film. The layered nature of the crystal structure provides numerous active surface sites and promotes efficient ion diffusion, making CuS particularly attractive for electrochemical energy-storage applications. One of the distinguishing features of CuS is the presence of intrinsic copper vacancies. These vacancies act as acceptor defects and are primarily responsible for the p-type conductivity observed in most CuS thin films. The high concentration of native defects results in a large hole concentration, which significantly enhances electrical conductivity. In addition, mixed-valence states of copper contribute to unusual electronic behavior that is intermediate between metallic and semiconducting conduction.

The electronic structure of CuS is governed mainly by hybridization between Cu 3d and S 3p orbitals. The valence band is dominated by copper 3d states with contributions from sulfur 3p orbitals, whereas the conduction band originates predominantly from sulfur orbitals with minor contributions from copper states. The overlap between these electronic states produces strong optical absorption across the visible region and contributes to efficient generation of charge carriers under illumination. The optical band gap of CuS reported in the literature generally lies between 1.2 and 2.5 eV, depending on deposition technique, crystallinity, particle size, stoichiometry, and measurement method. Thin films prepared by chemical bath deposition typically exhibit band-gap values in the range of 1.8–2.3 eV, while highly conductive Cu-rich films often display narrower apparent band gaps due to defect-related electronic states. The tunability of the band gap enables optimization of CuS for diverse applications such as solar energy conversion, photodetection, and photocatalysis.

Structurally, CuS thin films frequently exhibit preferred orientation along the (006), (103), (110), and (108) crystallographic planes. The relative intensity of these diffraction peaks depends strongly on deposition conditions and post-deposition heat treatment. Improved crystallinity generally leads to larger crystallite size, lower lattice strain, reduced dislocation density, and enhanced carrier mobility. The thermal stability of CuS is another important characteristic influencing device performance. At elevated temperatures, CuS may undergo phase transformation into copper-deficient sulfide phases if sulfur volatilization occurs. Consequently, annealing temperature and atmosphere must be carefully optimized to preserve the desired crystal structure while improving crystallinity and electrical conductivity. Annealing in sulfur-containing atmospheres is often employed to minimize sulfur loss and maintain stoichiometric composition. The chemical stability of CuS in ambient conditions is generally satisfactory, although prolonged exposure to oxidizing environments may produce thin oxide layers on the film surface. Appropriate encapsulation or surface passivation can significantly improve long-term stability, particularly for photovoltaic and photoelectrochemical applications [12-13].

3. Synthesis of CuS Thin Films by CBD method

CBD is one of the most widely used techniques for preparing CuS thin films because of its simplicity, low operating temperature, and cost-effectiveness. In this method, a clean substrate is immersed in an aqueous solution containing copper ions, sulfur ions, complexing agents, and pH-controlling reagents. The controlled release of metal and chalcogenide ions leads to the gradual formation of CuS nuclei on the substrate surface, resulting in uniform thin-film growth.

Copper salts such as copper chloride, copper nitrate, or copper sulfate are commonly employed as copper sources, while thiourea, thioacetamide, sodium sulfide, or sodium thiosulfate serve as sulfur precursors. Complexing agents including ethylenediaminetetraacetic acid (EDTA), triethanolamine (TEA), ammonia, sodium citrate, or tartaric acid regulate the concentration of free Cu^{2+} ions, thereby controlling the reaction rate and preventing rapid precipitation [14-15].

The overall deposition process generally involves the following steps like preparation of precursor solution, addition of the complexing agent, adjustment of solution pH, immersion of the cleaned substrate, controlled nucleation and crystal growth, washing and drying of the deposited film, post-deposition annealing when required. The growth mechanism is primarily governed by ion-by-ion deposition, although cluster-by-cluster deposition may also occur depending on supersaturation and solution chemistry. Slow ionic release promotes compact, uniform, and adherent films, whereas excessive supersaturation often produces porous or loosely attached deposits. Several deposition parameters influence film quality such as precursor concentration, deposition temperature, pH, deposition time, complexing agent concentration, stirring rate, substrate orientation and annealing temperature

Increasing deposition time generally increases film thickness until equilibrium is reached. Similarly, moderate deposition temperatures improve crystallinity by enhancing reaction kinetics, whereas excessively high temperatures may accelerate homogeneous precipitation within the solution. CBD offers several advantages, including low equipment cost, excellent substrate coverage, deposition on complex-shaped substrates, and compatibility with glass, silicon, fluorine-doped tin oxide (FTO), indium tin oxide (ITO), and flexible polymer substrates. However, the method may suffer from relatively slow deposition rates, sensitivity to solution chemistry, and possible incorporation of impurities if experimental conditions are not carefully optimized.

4. Properties of CuS Thin Films

4.1 Structural Properties

The structural properties of CuS thin films play a decisive role in determining their optical, electrical, electrochemical, and mechanical performance. These properties are primarily influenced by the deposition technique, precursor chemistry, substrate type, deposition temperature, solution pH, reaction time, and post-deposition annealing conditions. Variations in these parameters significantly affect the crystal structure, crystallite size, grain morphology, lattice strain, defect density, and film thickness, which ultimately govern the functional characteristics of the material.

Copper sulfide exists in several crystallographic phases depending on the Cu atomic ratio. Among these phases, covellite (CuS) is the most commonly reported structure for chemically deposited thin films. Covellite possesses a hexagonal crystal structure belonging to the space group $P6_3/mmc$. The layered arrangement of copper and sulfur atoms provides excellent electrical transport pathways and contributes to the high optical absorption observed in CuS thin films. X-ray diffraction studies generally reveal well-defined diffraction peaks corresponding to the hexagonal covellite phase. Depending on the deposition conditions, preferred orientation may occur along the (006), (101), (102), (103), (110), or (108) crystallographic planes. Films prepared under optimized conditions exhibit sharp and intense diffraction peaks, indicating improved crystallinity and phase purity. The average crystallite size is strongly dependent on synthesis conditions. Higher deposition temperatures and appropriate annealing treatments promote grain growth through atomic diffusion and recrystallization. Consequently, crystallite size generally increases with increasing annealing temperature, while lattice strain and dislocation density decrease. Larger crystallites reduce grain-boundary scattering, leading to improved electrical conductivity and enhanced carrier mobility [16-17].

Post-deposition annealing is widely employed to improve structural quality. Annealing promotes atomic rearrangement, reduces structural defects, relieves internal stress, and enhances crystallinity. However, excessive annealing temperatures may result in sulfur loss, phase

transformation, or oxidation, thereby deteriorating the structural integrity of the film. Therefore, optimization of annealing conditions is essential for maintaining phase stability while improving crystallinity.

Intrinsic defects also play an important role in determining the structural properties of CuS. Copper vacancies are the predominant native defects and contribute significantly to p-type conductivity. Although a moderate concentration of vacancies enhances electrical transport, excessive defect density may introduce localized states within the band gap and increase carrier recombination. Defect engineering through controlled synthesis and thermal treatment has therefore become an important strategy for improving the performance of CuS thin films.

4.2 Optical Properties

One of the most attractive characteristics of CuS is its high optical absorption coefficient in the visible and near-infrared regions. The absorption coefficient generally exceeds 10^4 cm^{-1}, enabling efficient harvesting of incident solar radiation even in relatively thin films. Such strong absorption makes CuS an excellent candidate for absorber layers in thin-film solar cells and photoelectrochemical devices. The optical absorption behavior is commonly investigated using UV–Visible spectroscopy. CuS thin films typically exhibit strong absorption in the wavelength range of 300–900 nm, with absorption gradually decreasing toward longer wavelengths. The exact absorption edge depends on deposition conditions and film composition.

Optical transmittance is another important parameter that determines the suitability of CuS for transparent or semi-transparent optoelectronic devices. Because CuS strongly absorbs visible light, transmittance is generally moderate to low within the visible region. However, thinner films often exhibit increased transparency due to reduced optical path length. Film thickness therefore provides an effective means of balancing transparency and light absorption depending on the intended application. The optical band gap is one of the most fundamental properties of CuS thin films. It represents the minimum energy required to excite an electron from the valence band to the conduction band. The band-gap energy is usually determined using Tauc plots obtained from UV–Visible absorption data. Reported band-gap values for CuS thin films generally range from approximately 1.2 to 2.5 eV, depending on synthesis technique, crystallinity, grain size, stoichiometry, and defect concentration [18-19].

Several factors contribute to band-gap variation. Nanocrystalline films often exhibit a slight widening of the band gap because of quantum confinement effects. Conversely, films containing a high concentration of defects or copper-rich compositions may exhibit narrower band gaps due to the formation of localized electronic states within the forbidden energy region. Post-deposition annealing frequently results in improved crystallinity and reduced defect density, leading to more well-defined optical absorption edges. The refractive index describes the propagation of light through CuS thin films and is strongly dependent on wavelength and film density. Highly

crystalline films generally possess larger refractive indices than poorly crystalline or porous films. Knowledge of the refractive index is important for designing optical coatings, multilayer interference filters, and antireflection coatings. The extinction coefficient is directly related to the attenuation of light within the material and is closely associated with the absorption coefficient. Larger extinction coefficients indicate stronger light absorption, which is advantageous for photovoltaic and photocatalytic applications where maximum photon utilization is desired. The dielectric properties of CuS are also important for electronic and optoelectronic device design. The complex dielectric constant consists of real and imaginary components representing energy storage and energy dissipation within the material, respectively. These parameters vary with photon energy and are influenced by free-carrier concentration and electronic polarization. Optical conductivity represents the ability of CuS to conduct charge carriers under optical excitation. It generally increases with photon energy because higher-energy photons generate a greater number of electron–hole pairs. Enhanced optical conductivity is beneficial for photoconductive devices and solar energy conversion systems. Another important optical parameter is the Urbach energy, which characterizes the width of localized electronic states near the band edge. Higher Urbach energy values indicate increased structural disorder and defect density within the material. Reduction of Urbach energy through improved crystallinity and optimized synthesis conditions generally enhances optical quality and reduces non-radiative recombination losses. Photoluminescence studies provide additional insight into the electronic structure of CuS thin films. Emission spectra arise from the radiative recombination of photogenerated electrons and holes. Defect-related emissions often appear because of copper vacancies, sulfur vacancies, or interstitial defects. Lower photoluminescence intensity generally indicates suppressed electron–hole recombination, which is advantageous for photocatalytic and photoelectrochemical applications. The optical response of CuS can be further improved through nanostructuring and heterostructure formation. Coupling CuS with wide-band-gap semiconductors such as ZnO or TiO_2 enhances light harvesting and promotes efficient charge separation. Similarly, incorporating carbon-based materials such as graphene or reduced graphene oxide improves carrier transport while reducing recombination losses.

4.3 Electrical Properties

The electrical properties of CuS thin films are of considerable importance because they directly influence the performance of photovoltaic devices, photoelectrochemical cells, photodetectors, gas sensors, and energy-storage systems. These properties are governed by several factors, including crystal structure, phase composition, film thickness, grain size, stoichiometry, defect concentration, and deposition conditions. Optimization of these parameters enables the fabrication of CuS thin films with improved electrical conductivity, carrier mobility, and charge transport characteristics.

CuS is generally recognized as a p-type semiconductor, primarily due to the presence of intrinsic copper vacancies. These vacancies act as acceptor defects, generating holes that serve as the majority charge carriers. The concentration of copper vacancies strongly influences the carrier concentration and, consequently, the electrical conductivity of the thin films. Controlled defect engineering is therefore an effective strategy for tailoring the electrical properties of CuS for specific applications. The electrical conductivity of CuS thin films varies over a wide range depending on the synthesis method and processing conditions. Films with improved crystallinity and larger grain size generally exhibit higher conductivity because grain-boundary scattering is reduced, allowing charge carriers to move more freely. Conversely, poorly crystalline films containing numerous structural defects exhibit lower conductivity owing to increased carrier trapping and scattering. Temperature-dependent conductivity measurements reveal the semiconducting nature of CuS thin films. In most cases, conductivity increases with increasing temperature, indicating thermally activated charge transport. At elevated temperatures, additional charge carriers gain sufficient thermal energy to overcome potential barriers at grain boundaries, resulting in enhanced electrical conduction.

5. Applications of CuS Thin Films

5.1 Solar Cells

One of the most important applications of CuS thin films is in photovoltaic devices. Their high absorption coefficient enables efficient absorption of sunlight within relatively thin absorber layers, reducing material consumption while maintaining excellent light-harvesting capability. CuS also possesses a suitable band gap for solar energy conversion and exhibits good electrical conductivity, facilitating efficient transport of photogenerated charge carriers. CuS thin films have been employed in several types of solar cells, including heterojunction, Schottky junction, and quantum dot-sensitized solar cells. They are frequently combined with n-type semiconductors such as CdS, ZnO, TiO_2, In_2S_3, and SnO_2 to form p–n heterojunctions. The internal electric field developed at the heterojunction interface promotes efficient separation of photogenerated electron–hole pairs and minimizes recombination losses.

The photovoltaic performance depends strongly on film crystallinity, thickness, morphology, and interface quality. Uniform films with compact grain structures generally exhibit lower series resistance and higher carrier mobility, resulting in improved short-circuit current density, open-circuit voltage, and overall conversion efficiency. Recent studies have demonstrated that nanostructured CuS films with hierarchical architectures provide enhanced light trapping and increased interfacial area, thereby improving photovoltaic performance. Surface passivation, interface engineering, and optimization of deposition parameters continue to play important roles in improving the efficiency and stability of CuS-based solar cells.

5.2 Photoelectrochemical Cells

CuS thin films are widely investigated as photoelectrodes for photoelectrochemical (PEC) cells because of their excellent visible-light absorption and favorable electrical properties. When illuminated, CuS generates electron–hole pairs that participate in electrochemical reactions at the semiconductor–electrolyte interface. The photocurrent generated by CuS photoelectrode depends on several factors, including crystal quality, carrier mobility, film thickness, electrolyte composition, and light intensity. Sulfide–polysulfide electrolytes are commonly employed because they improve electrode stability and suppress photocorrosion.

Nanostructured CuS films possessing porous or flower-like morphologies provide larger active surface areas and shorter diffusion paths for charge carriers, thereby increasing photocurrent density. The formation of heterojunctions with wide-band-gap semiconductors further enhances charge separation and significantly improves photoelectrochemical efficiency. CuS photoelectrode have also been investigated for photoelectrochemical water splitting and hydrogen generation. Although their conversion efficiency remains lower than that of some commercial semiconductor systems, continuous improvements in interface engineering, cocatalyst loading, and defect control have substantially enhanced their performance.

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SCIENTIFIC CONVERGENCE IN EMERGING TECHNOLOGIES: BRIDGING INTERDISCIPLINARY DISCOVERY AND SOCIETAL IMPACT

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Abstract

Scientific and technological progress is increasingly shaped by the convergence of disciplines, methods, data and emerging technologies. Complex challenges such as antimicrobial resistance, sustainable agriculture, environmental degradation, precision healthcare and responsible technology development cannot be addressed adequately through isolated disciplinary approaches. This chapter examines the meaning and evolution of convergence, distinguishes multidisciplinary, interdisciplinary and transdisciplinary approaches, and explains how problem-oriented integration can connect scientific discovery with proof of concept, technology development, validation, scale-up and societal application. Major domains including biotechnology and nanotechnology, artificial intelligence and biological sciences, computational biology, advanced materials, agriculture, environmental biotechnology and digital technologies are discussed. The chapter further considers emerging technologies, including AI, synthetic biology, high-throughput sequencing, robotics, additive manufacturing, digital twins and the Internet of Things, as enabling platforms for convergence. Key barriers include disciplinary communication, funding, infrastructure, data interoperability, reproducibility, ethics, regulation, intellectual property, commercialization and unequal access. Future directions emphasize autonomous experimentation, precision medicine, sustainable nanobiotechnology, One Health approaches to antimicrobial resistance, circular bioeconomy models, interdisciplinary education and responsible innovation. Overall, convergence is presented not merely as collaboration among disciplines but as deep integration organized around compelling scientific or societal problems.

Keywords: Scientific Convergence, Interdisciplinary Research, Emerging Technologies, Nanobiotechnology, Artificial Intelligence, Innovation, Technology Transfer, Green Synthesis, ZnO Nanoparticles, Sustainable Science.

1. Introduction

Science and technology have traditionally developed through specialized disciplines such as biology, chemistry, physics, mathematics, engineering, medicine, and computer science. This disciplinary specialization has played a fundamental role in generating detailed knowledge and establishing rigorous scientific methodologies. However, many of the major scientific and

societal challenges of the twenty-first century are complex and cannot be adequately addressed through the knowledge or tools of a single discipline. Challenges such as antimicrobial resistance, climate change, food and energy security, emerging infectious diseases, environmental pollution, cancer, neurological disorders, and sustainable manufacturing involve interconnected biological, physical, chemical, technological, and social dimensions. Consequently, increasing attention has been directed toward approaches that integrate knowledge and expertise across disciplinary boundaries (National Research Council, 2014; National Science Foundation, 2026).

The concept of convergence in science and technology represents a shift from isolated disciplinary research toward the deliberate integration of multiple areas of knowledge to address complex scientific and societal problems. The National Research Council described convergence as an approach to problem solving that cuts across disciplinary boundaries and integrates knowledge, tools, and ways of thinking from life and health sciences, physical and mathematical sciences, computational sciences, engineering, and related fields National Research Council (2014). Similarly, the National Science Foundation (NSF) characterizes convergence research as research driven by a specific and compelling problem that requires deep integration across disciplines National Science Foundation (2026).

1.1 Meaning of Convergence in Science and Technology

The term convergence generally refers to the coming together of previously distinct areas to form an integrated whole. In science and technology, convergence describes the systematic integration of knowledge, methods, tools, and expertise from different disciplines to address a shared research problem or societal need. It is therefore both a research strategy and an innovation pathway (National Research Council, 2014; National Science Foundation, 2026).

1.2 Evolution from Disciplinary to Interdisciplinary Research

The development of modern science has been strongly influenced by specialization. As scientific knowledge expanded, individual disciplines became increasingly subdivided into specialized fields. This process enabled researchers to develop sophisticated theories, methodologies, instruments, and experimental systems. However, increasing specialization also created boundaries between disciplines (National Research Council, 2014; National Science Foundation, 2026).

1.3 Need for Convergence in the Modern Scientific Era

The increasing complexity of contemporary scientific problems is one of the primary reasons for the growing importance of convergence. Problems such as antimicrobial resistance, precision medicine, sustainable agriculture, climate change, environmental remediation, and renewable energy involve multiple interacting variables and therefore require knowledge from several disciplines (National Research Council, 2014; National Science Foundation, 2026).

2. Concept of Convergence

Convergence is fundamentally an integrative approach to scientific problem solving. It recognizes that complex questions often exist at the interfaces between established disciplines and therefore require coordinated contributions from multiple areas of expertise. Rather than treating disciplines as isolated entities, convergence seeks to establish connections among them and create a unified framework for addressing a specific scientific or societal challenge (National Research Council, 2014; National Science Foundation, 2026).

The National Research Council (2014) identified convergence as an approach that integrates life sciences with physical, mathematical, computational, medical, engineering, and other areas of expertise. This integration can result in new conceptual frameworks, research tools, technologies, and applications. The process therefore involves both convergence of knowledge and convergence of people, institutions, technologies, and applications.

2.1 Convergence of Biology, Chemistry, Physics, Engineering and Computational Sciences

Biology and chemistry have long interacted through biochemistry and molecular biology. Contemporary convergence extends this relationship into areas such as synthetic biology, metabolic engineering, drug discovery, biomaterials, and biotechnology. Chemical principles are used to understand biological molecules, while biological systems can serve as platforms for producing valuable chemicals and materials (National Research Council, 2014; National Science Foundation, 2026).

2.2 Interdisciplinary and Transdisciplinary Approaches

Multidisciplinary research generally involves contributions from two or more disciplines toward a common topic or problem, while each discipline may retain its own concepts and methodologies. The researchers may work in parallel, and the findings are subsequently combined (National Research Council, 2014; National Science Foundation, 2026).

2.3 Discovery–Innovation–Application Continuum

A major strength of convergence is its ability to connect fundamental scientific discovery with innovation and practical application. Scientific discovery generates new knowledge about natural phenomena, biological systems, materials, processes, or mechanisms. However, discovery alone does not necessarily produce a useful technology. Translation requires additional stages involving validation, engineering, optimization, scale-up, regulatory evaluation, and implementation (National Research Council, 2014; National Science Foundation, 2026).

3. Major Domains of Scientific and Technological Convergence

Scientific and technological convergence is increasingly evident in research areas where the boundaries between traditional disciplines are becoming less distinct. Advances in instrumentation, computation, materials science, molecular biology, engineering, and data science have created opportunities for researchers to combine previously independent

approaches. The resulting integration can generate new knowledge, technologies, and applications that are difficult to achieve through isolated disciplinary research. The National Research Council identified convergence across life sciences, physical sciences, mathematics, computational sciences, medicine, engineering, and related fields as an important strategy for addressing complex scientific and societal challenges National Research Council (2014).

Several major domains illustrate the practical significance of convergence. These include biotechnology and nanotechnology, artificial intelligence and biological sciences, computational biology and medicine, advanced materials and healthcare, biotechnology and agriculture, and environmental science and engineering. These domains are not independent; rather, they increasingly overlap and form interconnected research and innovation ecosystems.

3.1 Biotechnology and Nanotechnology

The convergence of biotechnology and nanotechnology represents one of the most important examples of modern scientific integration. Biotechnology provides knowledge of biological molecules, cells, microorganisms, genes, enzymes, and biological processes, whereas nanotechnology provides tools for manipulating and engineering matter at the nanoscale. Their integration has contributed to the development of nanobiotechnology, nanomedicine, biosensors, drug-delivery systems, antimicrobial materials, diagnostic technologies, and advanced biomaterials (Roco & Bainbridge, 2003; El-Saadony *et al.,* 2024).

3.2 Artificial Intelligence and Biological Sciences

Artificial intelligence (AI) has emerged as a major enabling technology for scientific convergence. Machine learning and deep-learning approaches can process large datasets, identify patterns, generate predictions, and support decision-making. Their integration with biology has created rapidly developing areas such as computational biology, bioinformatics, AI-assisted drug discovery, protein structure prediction, genomics, systems biology, and precision medicine.

3.3 Computational Biology, Bioinformatics and Medicine

The convergence of computational science with biology and medicine has transformed the study of biological systems. Bioinformatics integrates biology, computer science, mathematics, and statistics to organize and analyze biological information. Computational biology extends this approach toward modelling biological processes and generating mechanistic hypotheses.

3.4 Advanced Materials, Engineering and Healthcare

The convergence of materials science, engineering, biology, and medicine has produced numerous technologies aimed at improving healthcare. Advanced materials can be designed to possess specific mechanical, chemical, electrical, optical, or biological properties. When these materials are engineered for interaction with biological systems, they become important components of biomedical technologies.

3.5 Biotechnology and Agriculture

Agriculture is another major area in which convergence can contribute to solving complex problems. Modern agricultural systems must simultaneously address food production, nutritional quality, climate variability, soil health, water availability, pests, diseases, and environmental sustainability.

3.6 Environmental Science, Biotechnology and Nanotechnology

Environmental biotechnology uses microorganisms, enzymes, plants, and biological processes for pollution control, wastewater treatment, bioremediation, and resource recovery. Nanotechnology can complement these approaches by providing advanced adsorbents, catalysts, sensors, membranes, and reactive materials (Roco & Bainbridge, 2003; El-Saadony *et al.,* 2024).

3.7 Convergence in Antimicrobial Resistance Research

Antimicrobial resistance (AMR) represents a particularly strong example of why scientific convergence is necessary. AMR is not exclusively a microbiological or medical problem. It involves microbial evolution, molecular biology, clinical medicine, pharmacology, epidemiology, environmental science, veterinary medicine, agriculture, public health, and policy.

4. From Scientific Discovery to Technological Application

Scientific progress does not end with the generation of new knowledge. The ultimate impact of many scientific discoveries depends on whether that knowledge can be translated into technologies, products, processes, policies, or interventions that address real-world needs. The journey from scientific discovery to practical application is therefore a complex process involving fundamental research, validation, technological development, optimization, scale-up, regulatory assessment, and implementation. Convergence in science and technology can facilitate this process by bringing together researchers from complementary disciplines at different stages of the innovation pathway, National Research Council (2014).

The relationship between science, technology, and innovation is not necessarily linear. Fundamental discoveries can stimulate technological development, while technological advances can provide new tools for scientific investigation. Similarly, practical societal problems can generate new research questions and redirect scientific discovery. Thus, modern innovation is better understood as a dynamic interaction between knowledge generation, technological development, application, and societal needs National Research Council (2014).

4.1 Scientific Discovery as the Foundation of Innovation

Scientific discovery refers to the generation of new knowledge concerning natural phenomena, biological systems, materials, mechanisms, processes, or relationships. Discovery-oriented research may be curiosity-driven or motivated by a specific scientific or societal problem (Li & Wang, 2024; Baaden *et al.,* 2024).

4.2 Knowledge Integration and Proof of Concept

The transition from discovery to application often begins with the integration of knowledge from multiple disciplines. Researchers must determine whether a scientific finding can be reproduced, whether the underlying mechanism is sufficiently understood, and whether it has potential practical value, National Research Council (2014).

4.3 Technology Development and Optimization

In nanotechnology, for example, small changes in synthesis conditions can influence particle size, morphology, surface chemistry, aggregation, and biological activity. Consequently, optimization requires simultaneous consideration of chemical and physical parameters and biological outcomes, National Research Council (2014).

4.4 Validation of Scientific and Technological Innovations

Validation is essential for determining whether an emerging technology performs consistently and safely under relevant conditions. Depending on the application, validation can involve laboratory experiments, animal studies, clinical studies, field trials, toxicological assessment, environmental evaluation, and comparison with existing technologies (Li & Wang, 2024; Baaden *et al.,* 2024).

4.5 Scale-Up and Translation

In biotechnology, additional challenges can arise because biological systems may exhibit variability. Microbial growth, enzyme production, metabolite secretion, and biological synthesis processes can be influenced by environmental and nutritional conditions, National Research Council (2014).

4.6 Commercialization and Technology Transfer

Commercialization represents the transition from a validated technology to a product, service, or process that can be implemented at scale. This stage may involve intellectual property protection, technology transfer, regulatory approval, manufacturing, market evaluation, investment, and partnerships with industry, National Research Council (2014).

4.7 Regulatory, Ethical and Safety Considerations

Scientific innovation must be accompanied by appropriate evaluation of safety, ethics, environmental consequences, and regulatory requirements. This is particularly important for technologies involving biological systems, nanoparticles, artificial intelligence, genetic engineering, and medical applications, National Research Council (2014).

4.8 Case Study: Green-Synthesized ZnO Nanoparticles as an Example of Convergence

Microbiology contributes to the selection and characterization of microorganisms capable of producing or facilitating nanoparticle synthesis. Biotechnology provides methods for cultivating biological systems and obtaining biologically active metabolites. Chemistry contributes to understanding precursor transformation and chemical reactions. Materials science and

nanotechnology are required to characterize nanoparticle size, morphology, crystallinity, surface chemistry, and stability. Microbiology and molecular biology can then be used to evaluate antimicrobial, antibiofilm, or antivirulence effects, National Research Council (2014).

4.8.1 Biological Synthesis of Nanoparticles

Fungal systems are particularly interesting because fungi can produce extracellular metabolites and enzymes that can participate in the transformation and stabilization of metal or metal-oxide nanoparticles. This creates an interface between microbiology and materials science, National Research Council (2014).

4.8.2 Physicochemical Characterization

Characterization is a critical stage in the translation of nanoparticle synthesis into a reproducible technology. Techniques such as ultraviolet-visible spectroscopy, Fourier-transform infrared spectroscopy, X-ray diffraction, transmission electron microscopy, dynamic light scattering, and zeta-potential analysis can provide complementary information, National Research Council (2014).

4.8.3 Biological Evaluation of ZnO Nanoparticles

After characterization, biological evaluation can determine whether the synthesized material possesses the intended biological activity. For antimicrobial applications, researchers may investigate bacterial growth inhibition, minimum inhibitory concentration, biofilm formation, metabolic activity, or specific virulence-associated properties.

4.8.4 Nanoparticles and Antivirulence Strategies

Traditional antimicrobial approaches primarily aim to inhibit or eliminate pathogenic microorganisms. In contrast, antivirulence strategies aim to reduce the ability of pathogens to cause disease by interfering with virulence-associated factors or pathways.

4.8.5 Computational Approaches in Nanobiotechnology

Computational methods can further strengthen the convergence framework. Molecular docking, molecular dynamics simulations, machine learning, and other computational approaches can be used to investigate potential interactions between nanoparticles, nanoparticle-associated molecules, microbial proteins, or therapeutic targets.

5. Role of Emerging Technologies in Scientific Convergence

Emerging technologies are transforming the way scientific research is conducted, interpreted, and translated into practical applications. Technologies such as artificial intelligence (AI), machine learning, nanotechnology, synthetic biology, bioinformatics, advanced imaging, robotics, additive manufacturing, and high-throughput sequencing are increasingly interconnected. Their convergence is creating new opportunities for scientific discovery while simultaneously accelerating the development of technologies for healthcare, agriculture, environmental protection, industrial biotechnology, and other sectors.

The increasing complexity and volume of scientific data have made technological integration essential. Modern research frequently requires the simultaneous use of experimental techniques, computational tools, advanced instrumentation, and data-analysis platforms. Consequently, emerging technologies should not be viewed as isolated innovations. Their greatest potential often emerges when they are combined with one another and integrated with established scientific disciplines National Research Council (2014).

5.1 Artificial Intelligence and Machine Learning

Artificial intelligence has become one of the most influential technologies supporting scientific convergence. AI refers broadly to computational systems capable of performing tasks associated with learning, prediction, pattern recognition, reasoning, and decision-making. Machine learning, a major component of AI, enables computational models to identify relationships in data and generate predictions without being explicitly programmed for every individual outcome (Pushkaran & Arabi, 2024; Zhang *et al.,* 2024).

5.2 Nanotechnology

Nanotechnology involves the understanding and manipulation of matter at the nanoscale and has become a major platform for scientific convergence. At the nanoscale, materials can exhibit physicochemical properties that differ substantially from their bulk counterparts. These properties can be exploited for applications in medicine, electronics, energy, agriculture, environmental remediation, and biotechnology (National Research Council, 2014; Roco & Bainbridge, 2003).

5.3 Synthetic Biology

Computational modelling and machine learning can further support synthetic biology by predicting biological pathway behavior and identifying optimal combinations of genes, enzymes, or regulatory elements. Experimental systems can then validate these computational predictions (National Research Council, 2014; Roco & Bainbridge, 2003).

5.4 Bioinformatics and High-Throughput Sequencing

The rapid development of sequencing technologies has fundamentally changed biological research. Modern sequencing platforms can generate enormous quantities of genomic information, requiring computational methods for storage, processing, analysis, and interpretation (National Research Council, 2014; Roco & Bainbridge, 2003).

5.6 Robotics and Laboratory Automation

Automation and robotics are increasingly being integrated into scientific research. Automated systems can perform repetitive experimental procedures with high precision and reproducibility. Laboratory automation can support high-throughput screening, sample preparation, liquid handling, microscopy, and data collection (National Research Council, 2014; Roco & Bainbridge, 2003).

5.16 Future Outlook

Emerging technologies are likely to become increasingly interconnected during the coming decades. Artificial intelligence may become integrated into laboratory automation, materials discovery, biotechnology, healthcare, and environmental monitoring. Nanotechnology may increasingly interact with synthetic biology and advanced manufacturing. Genomic data may be integrated with clinical and environmental information. Robotics may support automated experimentation, while cloud computing and large-scale data infrastructure will enable collaborative research across geographical boundaries (Pushkaran & Arabi, 2024; Zhang *et al.,* 2024).

5.17 Conclusion

Emerging technologies are powerful drivers of scientific and technological convergence. Artificial intelligence, nanotechnology, synthetic biology, bioinformatics, advanced imaging, robotics, additive manufacturing, IoT, and big-data technologies are increasingly interconnected with established scientific disciplines (Pushkaran & Arabi, 2024; Zhang *et al.,* 2024).

6. Challenges and Barriers to Scientific and Technological Convergence

Although convergence in science and technology provides substantial opportunities for discovery and innovation, its implementation is associated with several scientific, organizational, technological, ethical, economic, and regulatory challenges. Bringing together researchers from different disciplines does not automatically result in effective integration. Successful convergence requires shared objectives, compatible methodologies, appropriate infrastructure, interdisciplinary communication, sustained funding, and mechanisms for translating discoveries into practical outcomes, National Research Council (2014).

The complexity of convergent research is partly due to differences in scientific terminology, research cultures, methodological approaches, standards of evidence, and evaluation criteria. Researchers trained within highly specialized disciplines may have limited familiarity with concepts and techniques outside their primary field. Consequently, convergence requires not only multidisciplinary participation but also mechanisms that promote meaningful integration National Research Council (2014).

6.1 Disciplinary Boundaries and Communication Barriers

For example, a microbiologist may describe a research problem in terms of microbial growth, virulence, or cellular mechanisms, whereas a materials scientist may focus on surface chemistry, particle size, crystallinity, and material properties. An engineer may approach the same problem in terms of process optimization and scalability, while a computational scientist may frame it as a modelling or prediction problem (National Research Council 2014).

6.2 Differences in Research Methodologies

Different disciplines often use different research designs and standards for evidence. Laboratory sciences may prioritize controlled experiments and reproducibility, while computational fields may emphasize datasets, algorithms, predictive performance, and model validation (National Research Council 2014).

6.3 Institutional and Organizational Barriers

Interdisciplinary researchers may also face difficulties when their work does not fit neatly into conventional disciplinary categories. For example, a project combining microbiology, nanotechnology, computational biology, and materials science may be evaluated differently by reviewers from each field. National Research Council (2014).

6.4 Funding Challenges

Funding mechanisms may also be organized according to traditional disciplinary categories. Researchers may therefore find it difficult to obtain support for projects that do not fit clearly within one funding category (National Research Council 2014).

6.7 Reproducibility and Reliability

In nanotechnology, for example, differences in synthesis conditions can influence particle size, morphology, surface chemistry, aggregation, and biological activity. Similarly, computational models can produce different predictions depending on datasets, algorithms, parameters, and validation procedures (National Research Council 2014).

6.9 Safety and Environmental Concerns

Nanomaterials provide a useful example. Their small size and unique surface properties can provide useful biological and technological functions, but these same characteristics may influence interactions with cells, organisms, and ecosystems (National Research Council 2014).

6.19 Conclusion

Scientific and technological convergence offers significant opportunities for addressing complex problems, but its successful implementation requires overcoming substantial barriers. Disciplinary boundaries, communication difficulties, funding limitations, infrastructure requirements, data-integration problems, regulatory uncertainty, ethical concerns, and translation challenges can all limit the effectiveness of convergent research (National Research Council 2014).

7. Future Perspectives and Opportunities

The convergence of science and technology is expected to become increasingly important as scientific questions and societal challenges grow more complex. Advances in artificial intelligence, nanotechnology, biotechnology, genomics, advanced materials, robotics, computational science, and digital technologies are creating new opportunities for integration across traditionally separate disciplines. The future of scientific progress is therefore likely to

depend not only on deeper specialization but also on the ability to connect specialized knowledge in meaningful ways (National Research Council 2014).

Convergence has the potential to accelerate discovery, improve technological development, strengthen healthcare, support sustainable agriculture, address environmental challenges, and contribute to the development of new industries. However, realizing this potential will require appropriate infrastructure, interdisciplinary education, responsible governance, and stronger connections between research and application (National Research Council 2014).

7.1 Convergence-Driven Scientific Discovery

For example, improvements in computational power and artificial intelligence can facilitate biological discovery, while advances in biology can provide new targets for computational research. Similarly, advances in materials science can enable new biomedical technologies, while biological systems can inspire the development of novel materials (National Research Council 2014).

7.3 Convergence in Personalized and Precision Medicine

Healthcare represents one of the areas with the greatest potential for convergence. Future medical systems may increasingly integrate genomic information, molecular biomarkers, medical imaging, clinical records, wearable devices, artificial intelligence, and advanced therapeutic technologies (National Research Council 2014).

7.4 Future of Nanobiotechnology

The development of safer and more reproducible nanomaterials will be particularly important. Green and biological synthesis may also receive increasing attention because biological systems can provide alternative routes for nanoparticle synthesis and functionalization (National Research Council 2014).

7.5 Convergence in Antimicrobial Resistance Research

Antimicrobial resistance is expected to remain a major global health challenge. Addressing it will require integration across microbiology, molecular biology, medicinal chemistry, nanotechnology, computational science, clinical medicine, epidemiology, environmental science, and public health (World Health Organization, 2024; Bertagnolio *et al.,* 2024).

7.14 Convergence for Global Challenges

Many global challenges are interconnected. For example, climate change can affect agriculture, water availability, infectious disease patterns, and public health. Antimicrobial resistance can involve human health, animal health, agriculture, and environmental systems (National Research Council 2014).

Conclusion

The convergence of science and technology represents a fundamental transformation in the way scientific knowledge is generated, integrated, and translated into practical applications. While

traditional disciplinary research has provided the foundation for scientific advancement, the complexity of contemporary scientific and societal challenges increasingly requires knowledge and expertise from multiple disciplines. The future of science and technology is increasingly likely to be shaped by convergence. Artificial intelligence, biotechnology, nanotechnology, advanced materials, computational science, robotics, genomics, and digital technologies are creating new connections among previously separate disciplines (National Research Council, 2014). Convergence provides a framework for bringing together biology, chemistry, physics, engineering, mathematics, computational science, medicine, materials science, and emerging technologies around shared scientific or societal problems. Its importance lies not simply in the participation of multiple disciplines but in the deep integration of their concepts, methodologies, technologies, data, and expertise.

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