https://doi.org/10.30799/jacs.S208.26120308 J. Adv. Chem. Sci. – Volume 12 Issue 3 (2026) 960–964

ISSN: 2394-5311

Share Your Innovations through JACS Directory

Journal of Advanced Chemical Sciences

Visit Journal at https://www.jacsdirectory.com/jacs

Heterocyclic Systems in Modern Material Design: A Comprehensive Review

Savita M. Mathure[1],*, Gokul V. Surywanshi[1], Santosh S. Chobe[2], Tulshidas S. Savale[1],*

[1]Department of Chemistry, M.G.V's M.S.G. Arts, Science and Commerce College, Malegaon Camp, Malegaon, Nashik – 423 105, Maharashtra, India.
[2]Department of Chemistry, M.G.V.'s Loknete Vyankatrao Hiray Arts, Science and Commerce College, Panchavati, Nashik – 422 003, Maharashtra, India.

ARTICLEDETAILS

Article history:
Received 24 February 2026
Accepted 11 March 2026
Available online 14 April 2026

Keywords:
Heterocyclic Compounds
Functional Materials
Organic Semiconductors
Conducting Polymers
Material Science

ABSTRACT

Heterocyclic compounds represent a vital class of organic molecules that play a central role in the development of advanced functional materials. Characterized by the presence of heteroatoms such as nitrogen, oxygen, sulphur, and occasionally phosphorus or selenium within their ring structures, these compounds exhibit unique electronic, optical, and structural properties. The incorporation of heteroatoms significantly influences electron distribution, molecular polarity, aromaticity, and intermolecular interactions, resulting in distinctive physicochemical characteristics suitable for material design. Structurally, heterocyclic compounds are broadly classified into five-membered, six-membered, and fused ring systems, each displaying specific stability and electronic behaviour. Common examples include pyridine, pyrrole, thiophene, furan, imidazole, triazole, and quinoline derivatives. Their aromatic or partially aromatic nature enables effective charge delocalization, making them highly suitable for electronic and optoelectronic applications. In recent years, heterocyclic compounds have gained considerable importance in materials science due to their versatility and tunable properties. They are widely employed in organic electronics, energy storage devices, sensors, conducting polymers, photovoltaic systems, light-emitting devices, and high-performance coatings. Their compatibility with molecular engineering strategies allows precise control over structural and functional characteristics, facilitating the design of next-generation materials. Overall, heterocyclic compounds serve as essential building blocks bridging organic chemistry and modern technology. Ongoing advancements in synthetic methodologies and deeper insights into structure–property relationships continue to expand their applications. As materials science advances toward sustainable, flexible, and high-performance systems, heterocyclic compounds remain at the forefront of innovation and technological progress.

1. Introduction

Material science has undergone rapid and transformative development in recent decades, largely driven by the integration of organic chemistry into the design and fabrication of advanced functional materials [1]. Traditionally dominated by inorganic systems, material science now increasingly relies on organic and hybrid materials to meet the growing demand for lightweight, flexible, cost-effective, and sustainable technologies [2]. In this context, heterocyclic compounds have emerged as a cornerstone of modern material design due to their exceptional structural diversity, chemical versatility, and tunable physicochemical properties.

Heterocyclic compounds are defined as cyclic organic molecules in which one or more ring atoms are heteroatoms such as nitrogen, oxygen, sulfur, or, less commonly, phosphorus and selenium. The presence of these heteroatoms significantly alters the electronic distribution within the molecular framework, influencing properties such as polarity, aromaticity, redox behaviour, and intermolecular interactions [3]. As a result, heterocyclic systems exhibit a wide range of reactivities and functional characteristics that are not easily attainable with purely carbocyclic compounds [4].

One of the key advantages of heterocyclic compounds lies in their ability to participate in extended π-conjugation systems. This feature enables efficient charge delocalisation and transport, which are critical requirements for electronic and optoelectronic applications [5]. Nitrogen-containing heterocycles often act as electron donors or acceptors, sulphur-containing rings enhance charge mobility due to their high polarizability, and oxygen-containing heterocycles contribute to improved solubility and processability [6]. Such tunable electronic behaviour allows heterocyclic compounds to be precisely engineered for specific material functions.

The incorporation of heterocyclic motifs into functional materials has led to significant advancements in diverse technological areas, including organic semiconductors, light-emitting diodes, photovoltaic devices, electroactive polymers, sensors, and corrosion-resistant coatings. In organic electronics, heterocyclic compounds serve as essential components of organic field-effect transistors (OFETs), organic light-emitting diodes (OLEDs), and organic solar cells due to their favourable band gaps, thermal stability, and mechanical flexibility [7,8]. Their molecular structures can be systematically modified to optimise optical absorption, emission characteristics, and charge carrier mobility [9].

Beyond electronic applications, heterocyclic compounds play a vital role in enhancing material durability and performance. In protective coatings and surface engineering, heterocycle-based materials offer excellent corrosion resistance, chemical stability, and adhesion to metal surfaces [10]. In energy-related applications, heterocyclic frameworks contribute to improved electrochemical performance in batteries, supercapacitors, and electrocatalytic systems [11]. Additionally, their responsiveness to external stimuli makes them highly attractive for sensing and smart material applications [12].

One of the most significant aspects of heterocyclic compounds lies in their structure–property relationships. The nature and position of heteroatoms, degree of conjugation, substituent effects, and molecular planarity collectively determine the optical absorption, band gap, conductivity, thermal stability, and chemical robustness of the resulting materials. Nitrogen-containing heterocycles often exhibit strong electron-donating or electron-accepting behaviour, while sulphur-based heterocycles such as thiophenes enhance charge carrier mobility due to their high polarizability [13]. Oxygen-containing heterocycles contribute to improved solubility and processability, which are critical parameters for device fabrication.

In the realm of organic electronics, heterocyclic compounds serve as the core components of organic field-effect transistors (OFETs), organic light-emitting diodes (OLEDs), and organic photovoltaic cells (OPVs) [14]. Conjugated heterocyclic polymers and small molecules demonstrate excellent charge transport properties, tunable emission characteristics,

---

*Corresponding Author:savita1190@gmail.com(Savita M. Mathure)

https://doi.org/10.30799/jacs.S208.26120308

2394-5311 / JACS Directory©2026. This is an open access article licensed under CC BY 4.0.

Cite this Article as: Savita M. Mathure, Gokul V. Surywanshi, Santosh S. Chobe, Tulshidas S. Savale, Heterocyclic systems in modern material design: A comprehensive review, J. Adv. Chem. Sci. 12(3) (2026) 960–964.

and mechanical flexibility, enabling the development of lightweight, flexible, and cost-effective electronic devices [15]. Thiophene- and pyridine-based materials, in particular, have shown remarkable performance in semiconductor applications.

Heterocyclic compounds also play a vital role in energy storage and conversion technologies. In lithium-ion batteries, supercapacitors, and redox flow batteries, heterocyclic materials contribute to enhanced electrochemical stability, redox activity, and ion transport [16]. Nitrogen-rich heterocycles are widely used in electrode materials and electrolytes due to their strong coordination ability and favourable redox behaviour. Additionally, heterocyclic frameworks are increasingly explored in electrocatalysis and photocatalysis for hydrogen evolution, oxygen reduction, and carbon dioxide reduction reactions [17].

Overall, the unique combination of structural flexibility, functional tunability, and broad applicability positions heterocyclic compounds as indispensable components in contemporary material science. A deeper understanding of their synthesis, structure–property relationships, and integration into functional systems continues to drive innovation in next-generation materials. This chapter aims to provide a comprehensive overview of heterocyclic compounds as functional materials, highlighting their synthesis strategies, fundamental properties, and expanding role in advanced material science applications.

2. Classification of Heterocyclic Compounds

Heterocyclic compounds (Table 1) can be broadly classified based on ring size, type and number of heteroatoms, and aromaticity. Common five-membered heterocycles include pyrrole, furan, and thiophene, while six-membered heterocycles include pyridine, pyrimidine, and pyrazine. Fused heterocyclic systems such as indole, benzothiophene, and quinoline are also of significant importance in material applications.

Table 1 Heterocyclic compounds type and examples

Type	Examples	Material Applications
Five-membered	Pyrrole, Thiophene	OLEDs, Conducting polymers
Six-membered	Pyridine, Pyrimidine	Sensors, Energy storage
Fused systems	Indole, Quinoline	Organic electronics, Photovoltaic [18]

Heterocyclic compounds constitute a broad and diverse class of organic molecules, and their classification is essential for understanding their structural features, chemical behaviour, and functional relevance in material science. Based on ring size, nature and number of heteroatoms, degree of saturation, and structural complexity, heterocyclic compounds can be systematically categorised into several classes. Such classification not only facilitates rational molecular design but also aids in correlating structure with material properties.

2.1 Classification Based on Ring Size

One of the most fundamental approaches to classifying heterocyclic compounds is based on the size of the ring system.

Five-membered heterocycles typically contain one or more heteroatoms and often exhibit aromatic or partially aromatic character. Common examples include pyrrole, furan, thiophene, imidazole, oxazole, and thiazole. These compounds are particularly significant in material science due to their strong π-conjugation and high chemical stability. Thiophene and its derivatives, for instance, are extensively used in conducting polymers and organic semiconductors because of their excellent charge transport properties [19].

Six-membered heterocycles include compounds such as pyridine, pyrimidine, pyrazine, and triazine. These systems generally show greater thermal and chemical stability compared to five-membered rings. Nitrogen-containing six-membered heterocycles are widely employed as electron-deficient units in optoelectronic materials, coordination polymers, and energy storage devices [20].

Large-ring heterocycles or macrocyclic systems contain more than six atoms in the ring and include porphyrins, phthalocyanines, and crown ethers. These compounds exhibit unique electronic, magnetic, and coordination properties and find applications in catalysis, sensing, photodynamic materials, and solar energy conversion [21].

2.2 Classification Based on Nature and Number of Heteroatoms

Heterocyclic compounds can also be classified according to the type and number of heteroatoms present in the ring. Monoheterocyclic compounds contain only one heteroatom, such as nitrogen in pyridine, oxygen in furan, or sulphur in thiophene. These compounds often serve as fundamental building blocks in material synthesis and polymer design [22]. Diheterocyclic compounds contain two heteroatoms, which may be identical or different. Examples include imidazole (two nitrogen atoms), oxazole (one oxygen and one nitrogen), and thiazole (one sulfur and one nitrogen). The presence of multiple heteroatoms enhances intermolecular interactions, coordination ability, and electronic tunability [23]. Polyheterocyclic compounds possess three or more heteroatoms within the ring system, such as triazoles and tetrazines. These compounds are particularly important in high-performance materials due to their strong electron-withdrawing character, thermal stability, and redox activity [24].

2.3 Classification Based on Degree of Saturation

Based on the saturation level of the ring, heterocyclic compounds can be divided into saturated, partially saturated, and fully unsaturated systems. Saturated heterocycles, such as tetrahydrofuran and piperidine, lack π-electron delocalisation and primarily exhibit insulating behaviour [3]. However, they are valuable in polymer backbones and as flexible linkers in functional materials. Partially saturated heterocycles contain both single and double bonds, offering moderate electronic delocalisation. These compounds often serve as intermediates in material synthesis [25]. Aromatic heterocycles are fully unsaturated and obey Hückel's rule, resulting in high stability and extensive π-conjugation. Aromatic heterocycles such as thiophene, pyridine, and indole are of paramount importance in electronic, optoelectronic, and sensing applications [5].

2.4 Classification Based on Structural Complexity

Heterocyclic compounds may also be categorised based on the complexity of their molecular framework. Simple heterocycles consist of a single ring system and serve as core units in material design. Fused heterocyclic systems contain two or more rings sharing common atoms, such as indole, quinoline, benzothiazole, and carbazole. These compounds exhibit enhanced conjugation and rigidity, leading to improved optical absorption, charge mobility, and thermal stability. Bridged and spiro heterocycles represent advanced structural motifs that introduce three-dimensionality and mechanical robustness, making them suitable for high-performance polymers and advanced coatings [26].

2.5 Functional Classification in Material Science

From a material science perspective, heterocyclic compounds can also be classified based on their functional roles.

- Electron-donating heterocycles, such as pyrrole and thiophene, are widely used in conducting polymers [27].
- Electron-accepting heterocycles, such as pyridine and triazine, are essential in organic photovoltaics and n-type semiconductors [28].
- Redox-active heterocycles play a key role in energy storage and electrochemical applications [29].
- Coordination-capable heterocycles are crucial in metal–organic frameworks (MOFs) and hybrid materials [30].

This systematic classification highlights the structural and functional diversity of heterocyclic compounds and underscores their central role in the rational design of advanced functional materials. A clear understanding of these categories provides the foundation for exploring synthesis strategies, structure–property relationships, and application-specific material performance in subsequent sections.

3. Synthesis Methods of Heterocyclic Compounds

The synthesis of heterocyclic compounds is a cornerstone of organic and materials chemistry, as the performance of heterocycle-based materials strongly depends on molecular structure, purity, and functional group distribution [31]. Over the years, a wide range of synthetic strategies has been developed to construct heterocyclic frameworks with controlled ring size, heteroatom composition, and substitution patterns. Advances in synthetic methodologies have not only improved reaction efficiency and selectivity but have also enabled the development of sustainable and scalable processes suitable for material applications.

3.1 Classical Synthetic Approaches

Traditional methods for heterocycle synthesis remain widely used due to their simplicity, reliability, and adaptability to large-scale production [32]. Cyclisation reactions form the basis of many classical heterocyclic syntheses, where linear or branched precursors undergo intramolecular bond formation to generate ring systems. Examples include the Paal–Knorr synthesis for five-membered heterocycles such as pyrroles, furans, and thiophenes, and the Hantzsch synthesis for nitrogen-containing heterocycles [33]. These methods offer straightforward routes to aromatic heterocycles with good yields and structural predictability. Condensation

https://doi.org/10.30799/jacs.S208.26120308

Cite this Article as: M. Mathure, Gokul V. Surywanshi, Santosh S. Chobe, Tulshidas S. Savale, Heterocyclic systems in modern material design: A comprehensive review, J. Adv. Chem. Sci. 12(3) (2026) 960–964.

reactions are extensively employed for the construction of six-membered heterocycles. Reactions such as the Knoevenagel and Biginelli condensations allow the formation of heterocyclic cores under relatively mild conditions. These strategies are particularly useful for synthesising functionalized heterocycles with tunable electronic properties required for optoelectronic and sensing materials [13]. Rearrangement reactions, including ring expansion and contraction processes, also play an important role in heterocycle synthesis. These reactions enable access to structurally complex heterocycles that may be difficult to obtain through direct cyclisation routes [25].

3.2 Multicomponent Reactions (MCRs)

Multicomponent reactions have gained significant attention as efficient and atom-economical strategies for heterocycle synthesis. In these reactions, three or more reactants combine in a single step to form complex heterocyclic products. MCRs offer several advantages, including reduced reaction time, minimal waste generation, and high structural diversity. The Ugi, Passerini, and Biginelli reactions are widely used multicomponent approaches for synthesising nitrogen-rich heterocycles [34]. These methods are particularly attractive for material science applications, as they enable rapid screening of functional heterocyclic libraries for electronic, optical, or electrochemical properties.

3.3 Metal-Catalysed and Cross-Coupling Strategies

Metal-catalysed reactions have revolutionised heterocyclic synthesis by providing high regioselectivity, functional group tolerance, and scalability. Transition-metal-catalysed cross-coupling reactions such as Suzuki–Miyaura, Stille, Heck, and Sonogashira reactions are extensively employed to construct conjugated heterocyclic systems [35]. These methods are especially important for the synthesis of π-conjugated heterocyclic polymers and oligomers used in organic electronics, photovoltaics, and sensing devices. Palladium-, nickel-, and copper-catalysed reactions allow precise control over molecular architecture, enabling the optimisation of charge transport and optical properties.

3.4 Polymerisation and Self-Assembly Approaches

In material science, heterocyclic compounds are often synthesised not only as small molecules but also as polymeric or supramolecular systems. Chemical and electrochemical polymerisation techniques are commonly used to produce conducting polymers such as polythiophene, polypyrrole, and polyaniline. These methods offer control over molecular weight, doping level, and film morphology, which directly influence electrical conductivity and mechanical properties [36]. Self-assembly strategies, driven by non-covalent interactions such as hydrogen bonding, π–π stacking, and metal coordination, enable the formation of ordered heterocyclic nanostructures. Such approaches are particularly valuable for fabricating thin films, nanowires, and porous materials for advanced applications.

3.5 Green and Sustainable Synthetic Methods

The growing emphasis on sustainability has led to the development of environmentally benign synthesis strategies for heterocyclic compounds. Microwave-assisted synthesis significantly reduces reaction time and energy consumption while improving yields and selectivity. Solvent-free and aqueous-phase reactions minimise the use of hazardous organic solvents. Biocatalytic and enzyme-mediated reactions offer mild reaction conditions and high selectivity [37]. These green approaches are increasingly adopted for the synthesis of heterocyclic materials intended for large-scale industrial applications, aligning material development with environmental and economic considerations.

3.6 Post-Synthetic Functionalization

Post-synthetic modification is a powerful strategy for tuning the properties of heterocyclic materials. Functional groups can be introduced or modified after ring formation to adjust solubility, electronic behaviour, and surface affinity. This approach is particularly useful in the design of heterocycle-based polymers, coatings, and hybrid materials where fine control over functionality is required [20].

In summary, the diverse range of synthetic strategies available for heterocyclic compounds enables precise control over molecular structure and functionality. The continuous evolution of classical, modern, and green synthesis techniques has significantly expanded the scope of heterocyclic materials in advanced technological applications. A thorough understanding of these synthetic approaches provides the foundation for tailoring heterocyclic compounds to meet the specific demands of next-generation material science.

4. Applications of Heterocyclic Compounds in Material Science

Heterocyclic compounds play a crucial role in material science due to their unique electronic configurations, structural flexibility, and ability to form extended π-conjugated systems. The presence of heteroatoms such as nitrogen, oxygen, and sulphur enable fine control over electronic, optical, thermal, and chemical properties, making these compounds indispensable in a wide range of advanced material applications. Their versatility has led to significant technological advancements in electronics, energy systems, coatings, sensors, and hybrid materials [38].

4.1 Organic Electronics and Optoelectronic Devices

One of the most prominent applications of heterocyclic compounds is in organic electronics. Conjugated heterocycles such as thiophene, pyrrole, carbazole, and pyridine derivatives serve as the core components of organic semiconductors. These materials exhibit high charge carrier mobility, tunable band gaps, and mechanical flexibility, which are essential for organic field-effect transistors (OFETs), organic light-emitting diodes (OLEDs), and organic photovoltaic (OPV) devices [39]. Heterocyclic compounds contribute significantly to light emission and absorption processes. Nitrogen-containing heterocycles enhance electron-transport properties, while sulphur-based heterocycles improve hole mobility. The ability to tailor emission colour, efficiency, and stability through molecular engineering makes heterocyclic materials highly attractive for next-generation display and lighting technologies.

4.2 Energy Storage and Conversion Systems

Heterocyclic compounds are increasingly employed in energy-related materials due to their redox activity, electrochemical stability, and ion-coordination capability. In lithium-ion batteries and supercapacitors, heterocyclic frameworks are used as electrode materials, electrolytes, and conductive additives. Nitrogen-rich heterocycles improve charge storage capacity and cycling stability by facilitating electron transfer and ion transport [40]. In energy conversion applications, heterocyclic compounds play a vital role in electrocatalysis and photocatalysis. Heterocycle-based materials are explored for hydrogen evolution, oxygen reduction, and carbon dioxide reduction reactions. Their tunable electronic structure allows optimisation of catalytic activity and selectivity, contributing to the development of sustainable energy technologies [41].

4.3 Conducting Polymers and Electroactive Materials

Conducting polymers derived from heterocyclic monomers such as thiophene, pyrrole, and aniline are widely used in electroactive materials. Polythiophene, polypyrrole, and polyaniline exhibit excellent electrical conductivity, environmental stability, and processability. These materials are employed in flexible electronics, electromagnetic shielding, smart textiles, and antistatic coatings [42]. The electrochemical responsiveness of heterocyclic polymers enables their use in actuators, sensors, and controlled drug delivery systems. Their ability to undergo reversible oxidation and reduction processes makes them ideal for stimuli-responsive and smart material applications.

4.4 Sensors and Detection Technologies

Heterocyclic compounds are highly effective in sensing applications due to their strong interaction with chemical and biological analytes. Changes in conductivity, fluorescence, or colour upon analyte binding form the basis of heterocycle-based sensors [43]. These materials are widely used for gas sensing, humidity detection, and the detection of metal ions and toxic pollutants. Nitrogen- and sulfur-containing heterocycles exhibit high affinity toward gases such as ammonia, nitrogen dioxide, and volatile organic compounds, enabling sensitive and selective detection. Their fast response time and low detection limits make them suitable for environmental monitoring and industrial safety applications.

4.5 Protective Coatings and Corrosion-Resistant Materials

In surface engineering and coatings, heterocyclic compounds offer excellent corrosion resistance, thermal stability, and chemical durability. Heterocycle-based inhibitors form strong coordination bonds with metal surfaces, creating protective layers that prevent oxidation and degradation. These materials are widely used in aerospace, marine, and industrial infrastructure applications. Heterocyclic polymers and composites are also employed as high-performance coatings for electronic devices, providing insulation, moisture resistance, and mechanical protection. Their strong adhesion and long-term stability contribute to enhanced material lifespan [44].

Cite this Article as: M. Mathure, Gokul V. Surywanshi, Santosh S. Chobe, Tulshidas S. Savale, Heterocyclic systems in modern material design: A comprehensive review, J. Adv. Chem. Sci. 12(3) (2026) 960–964.

4.6 Hybrid, Nanostructured, and Framework Materials

Recent advances in material science have focused on integrating heterocyclic compounds into hybrid and nanostructured materials. Heterocycles serve as organic linkers in metal–organic frameworks (MOFs) and covalent organic frameworks (COFs), imparting porosity, structural stability, and functional tunability [45]. These materials find applications in gas storage, separation, catalysis, and sensing. Heterocyclic nanocomposites combine organic functionality with inorganic components such as metal oxides, nanoparticles, and carbon-based materials. Such hybrid systems exhibit enhanced mechanical strength, electrical conductivity, and multifunctionality, making them promising candidates for advanced technological applications. The broad spectrum of applications of heterocyclic compounds highlights their indispensable role in modern material science. Their structural diversity, electronic tunability, and functional adaptability enable the development of high-performance materials for electronics, energy, sensing, and protective technologies. Continued research and innovation in heterocyclic material design are expected to drive significant advancements in sustainable and next-generation material systems [46].

5. Conclusion

Heterocyclic compounds represent a versatile and indispensable class of materials in modern material science. Their unique structural features, tunable electronic properties, and wide-ranging applications underscore their importance in advanced technologies. Continued research into sustainable synthesis, structure–property relationships, and multifunctional heterocyclic systems is expected to drive future innovations in functional materials.

Heterocyclic compounds have firmly established themselves as indispensable components in the field of material science due to their exceptional structural diversity, electronic versatility, and functional adaptability. The incorporation of heteroatoms such as nitrogen, oxygen, and sulfur within cyclic frameworks significantly alters molecular electronic distribution, enabling precise tuning of physicochemical properties that are crucial for advanced material applications. As a result, heterocyclic compounds bridge fundamental organic chemistry with cutting-edge material engineering.

The systematic classification of heterocyclic compounds based on ring size, heteroatom composition, saturation level, and structural complexity provides a strong foundation for rational material design. Advances in synthetic strategies ranging from classical cyclisation and condensation reactions to modern metal-catalysed, multicomponent polymerisation and green chemistry approaches have enabled the efficient construction of complex heterocyclic architectures with controlled functionality and scalability. These developments have expanded the scope of heterocyclic compounds from small molecules to polymers, frameworks, and hybrid nanomaterials.

A critical understanding of structure–property relationships has revealed how heterocyclic frameworks govern key material characteristics such as charge transport, optical response, thermal stability, and electrochemical activity. This insight has driven their successful integration into a wide range of applications, including organic electronics, optoelectronic devices, energy storage and conversion systems, sensors, corrosion-resistant coatings, and smart materials. The versatility of heterocyclic compounds in fulfilling diverse functional roles underscores their central importance in both established and emerging technologies.

Looking ahead, the continued evolution of sustainable synthesis methods, molecular engineering strategies, and hybrid material systems is expected to further enhance the performance and applicability of heterocyclic materials. As material science increasingly prioritises efficiency, flexibility, and environmental responsibility, heterocyclic compounds are poised to play a pivotal role in shaping next-generation functional materials. Their continued exploration will undoubtedly contribute to innovative solutions for contemporary technological and societal challenges.

References

[1] L. Nicole, C. Laberty-Robert, L. Rozes, C. Sanchez, Hybrid materials science: a promised land for the integrative design of multifunctional materials, Nanoscale 6 (2014) 6267–6292.
[2] Z. Ren, Y. Ke, M.A. McCarthy, D.J. Lipomi, Flexible sensors based on organic-inorganic hybrid materials, Adv. Mat. Tech. 6 (2021) 2000889.
[3] A.T. Balaban, D.C. Oniciu, A.R. Katritzky, Aromaticity as a cornerstone of heterocyclic chemistry, Chem. Rev. 104 (2004) 2777–2812.
[4] F. De Proft, P. Geerlings (Eds.), Structure, bonding and reactivity of heterocyclic compounds, Vol. 38, Springer, Berlin, 2014.
[5] R. Iftikhar, F.Z. Khan, N. Naeem, Recent synthetic strategies of small heterocyclic organic molecules with optoelectronic applications: a review, Mol. Divers. 28 (2024) 271–307.
[6] N.N. Makhova, V.V. Alekseev, A.K. Buryak, A.A. Shcherbakov, Progress in the chemistry of nitrogen-, oxygen- and sulfur-containing heterocyclic systems, Russ. Chem. Rev. 89 (2020) 55–124.
[7] H. Bronstein, C.B. Nielsen, B.C. Schroeder, I. McCulloch, The role of chemical design in the performance of organic semiconductors, Nat. Rev. Chem. 4 (2020) 66–77.
[8] J.E. Anthony, Functionalized acenes and heteroacenes for organic electronics, Chem. Rev. 106 (2006) 5028–5048.
[9] B.K. Yap, R. Xia, M. Campoy-Quiles, P.N. Stavrinou, D.D.C. Bradley, Simultaneous optimization of charge-carrier mobility and optical gain in semiconducting polymer films, Nat. Mater. 7 (2008) 376–380.
[10] L.K.M.O. Goni, L. Guo, D.Q. Kong, G.Q. Li, Bioinspired heterocyclic compounds as corrosion inhibitors: a comprehensive review, Chem. Asian J. 16 (2021) 1324–1364.
[11] X. Feng, H. Zhang, Q. Chen, J. Zhang, Y. Liu, Untangling the respective effects of heteroatom-doped carbon materials in batteries, supercapacitors and the ORR to design high performance materials, Energy Environ. Sci. 14 (2021) 2036–2089.
[12] M. Mrinalini, S. Prasanthkumar, Recent advances on stimuli-responsive smart materials and their applications, ChemPlusChem 84 (2019) 1103–1121.
[13] A. Bhardwaj, P. Singh, V. Kumar, R. Singh, Naphthalene diimide-annulated heterocyclic acenes: synthesis, electrochemical and semiconductor properties and their multifaceted applications, Chem. Eur. J. 30 (2024) e202400208.
[14] G.A. Nowsherwan, Z.W. Wang, J.P. Liu, Y. Chen, Advances in organic materials for next-generation optoelectronics: potential and challenges, Organics 5 (2024) 520–560.
[15] P. Palani, S. Karpagam, Conjugated polymers – a versatile platform for various photophysical, electrochemical and biomedical applications: a comprehensive review, New J. Chem. 45 (2021) 19182–19209.
[16] Y. Zhao, Y. Ding, J. Song, G. Li, G. Yu, A chemistry and material perspective on lithium redox flow batteries towards high-density electrical energy storage, Chem. Soc. Rev. 44 (2015) 7968–7996.
[17] P. Prabhu, V. Jose, J.M. Lee, Heterostructured catalysts for electrocatalytic and photocatalytic carbon dioxide reduction, Adv. Funct. Mater. 30 (2020) 1910768.
[18] N. Neha, S. Kashyap, N. Nikita, A. Singh, U. Narang, et al., Unlocking the versatility of meso-substituted heterocyclic BODIPY: A comprehensive review across diverse applications, ChemSelect 10(38) (2025) e04534.
[19] G. Turkoglu, M.E. Cinar, T. Ozturk, Thiophene-based organic semiconductors, in: Sulfur Chemistry, Springer, Cham, Switzerland, 2017, pp.79–123.
[20] J. Huang, G. Yu, Structural engineering in polymer semiconductors with aromatic N-heterocycles, Chem. Mater. 33(5) (2021) 1513–1539.
[21] I.V. Lightcap, P.V. Kamat, Graphitic design: prospects of graphene-based nanocomposites for solar energy conversion, storage, and sensing, Acc. Chem. Res. 46(10) (2013) 2235–2243.
[22] D.A. Tomalia, Birth of a new macromolecular architecture: dendrimers as quantized building blocks for nanoscale synthetic polymer chemistry, Prog. Polym. Sci. 30(3–4) (2005) 294–324.
[23] Z. Qi, Y. Zhou, R. Guan, Y. Fu, J.B. Baek, Tuning the coordination environment of carbon-based single-atom catalysts via doping with multiple heteroatoms and their applications in electrocatalysis, Adv. Mater. 35 (2023) 2210575.
[24] Y. Ding, C. Zhang, L. Zhang, Y. Zhou, G. Yu, Molecular engineering of organic electroactive materials for redox flow batteries, Chem. Soc. Rev. 46 (2017) 270–282.
[25] I. Nakamura, Y. Yamamoto, Transition-metal-catalyzed reactions in heterocyclic synthesis, Chem. Rev. 104(5) (2004) 2127–2198.
[26] E.M. Carreira, T.C. Fessard, Four-membered ring-containing spirocycles: synthetic strategies and opportunities, Chem. Rev. 114(16) (2014) 8257–8322.
[27] N.J.L. Guernion, W. Hayes, 3- and 3,4-substituted pyrroles and thiophenes and their corresponding polymers: A review, Curr. Org. Chem. 8 (2004) 2263–2300.
[28] C. Mathur, R. Gupta, R.K. Bansal, Organic donor-acceptor complexes as potential semiconducting materials, Chem. Eur. J. 29 (2023) e202304139.
[29] G. Kwon, Y. Ko, Y. Kim, K. Kim, K. Kang, Versatile redox-active organic materials for rechargeable energy storage, Acc. Chem. Res. 54 (2021) 2927–2938.
[30] F.A.A. Paz, J. Klinowski, S.M.F. Vilela, J.P.C. Tomé, J.A.S. Cavaleiro, et al., Ligand design for functional metal-organic frameworks, Chem. Soc. Rev. 41 (2012) 1088–1110.
[31] A.R. Mahmoud, Heterocyclic compounds in modern drug design: synthetic strategies and biological targets, Ph.D. thesis, Shorouk Academy, Egypt, 2025.
[32] K. Lovato, P.S. Fier, K.M. Maloney, The application of modern reactions in large-scale synthesis, Nat. Rev. Chem. 5(8) (2021) 546–563.
[33] N. Kaur, P. Bhardwaj, M. Gupta, Recent developments in the synthesis of five- and six-membered N-heterocycles from dicarbonyl compounds, Curr. Org. Chem. 25(22) (2021) 2765–2790.
[34] R.L. Mohlala, T.J. Rashamuse, E.M. Coyanis, Highlighting multicomponent reactions as an efficient and facile alternative route in the chemical synthesis of organic-based molecules: a tremendous growth in the past 5 years, Front. Chem. 12 (2024) 1469677.
[35] J.I. Ayogu, E.A. Onoabedje, Recent advances in transition metal-catalysed cross-coupling of (hetero)aryl halides and analogues under ligand-free conditions, Catal. Sci. Technol. 9(19) (2019) 5233–5255.
[36] D. Sarmah, Studies on the palladium and copper catalysed synthesis of some functionalised carbocycles and heterocycles, Ph.D. thesis, Tezpur University, 2025.

Cite this Article as: M. Mathure, Gokul V. Surywanshi, Santosh S. Chobe, Tulshidas S. Savale, Heterocyclic systems in modern material design: A comprehensive review, J. Adv. Chem. Sci. 12(3) (2026) 960–964.

[37] J. Starvaggi, R. Ettari, Microwave-assisted organic synthesis: an eco-friendly method of green chemistry, Pharmaceuticals 18(11) (2025) 1692.

[38] H.R. Lim, H.S. Kim, R. Qazi, Y.-T. Kwon, J.-W. Jeong, et al., Advanced soft materials, sensor integrations, and applications of wearable flexible hybrid electronics in healthcare, energy, and environment, Adv. Mater. 31(48) (2019) 1900924.

[39] J.W. Lim, Polymer materials for optoelectronics and energy applications, Materials 17(15) (2024) 3698.

[40] Q. Yu, Z. Xue, M. Li, P. Qiu, C. Li, et al., Electrochemical activity of nitrogen-containing groups in organic electrode materials and related improvement strategies, Adv. Energy Mater. 10(35) (2020) 2002523.

[41] J. Wang, S. Dou, X. Wang, Structural tuning of heterogeneous molecular catalysts for electrochemical energy conversion, Sci. Adv. 7(13) (2021) eabf3989.

[42] K. Althagafy, F.A. Alamer, Metal-coated textiles in composite materials: advances in manufacturing techniques, properties, and applications, Cellulose 32(9) (2025) 5709–5733.

[43] D. Udhayakumari, A. Nanthakumar, Fluoride ion detection with heterocyclic chromogenic and fluorogenic probes: molecular design and response pathways, J. Fluor. Chem. 290 (2026) 110543.

[44] Z.H. Zhao, P.C. Zhao, Y. Zhao, J.L. Zuo, C.H. Li, An underwater long-term strong adhesive based on boronic esters with enhanced hydrolytic stability, Adv. Funct. Mater. 32(18) (2022) 2111959.

[45] C. Qian, Y. Zhao, Engineering heterocyclic linkages to expand the structural and functional diversity of covalent organic frameworks, Angew. Chem. Int. Ed. 64(5) (2025) e202516352.

[46] A. Boretti, B. Banik, A narrative review of four-membered heterocycles in next-generation energy conversion and storage, Energy Sci. Eng. 13(2) (2025) 701–715.

Special Issue Publication Statement

This article is included in the Special Issue of the journal comprising peer-reviewed papers selected from the International Conference on “Frontiers in Chemical and Material Sciences (ICFCMS-2026)”, held on 3rd and 4th February 2026 at MGV's Maharaja Sayajirao Gaikwad Arts, Science and Commerce College, Malegaon Camp, Malegaon, Nashik – 423 105, Maharashtra, India.

https://doi.org/10.30799/jacs.S208.26120308

Cite this Article as: M. Mathure, Gokul V. Surywanshi, Santosh S. Chobe, Tulshidas S. Savale, Heterocyclic systems in modern material design: A comprehensive review, J. Adv. Chem. Sci. 12(3) (2026) 960–964.