



Recent Advances in Engineering Aromatic Frameworks having Benzene Derivatives to Functional Polycyclic Aromatic Materials

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Abstract: Aromatic compounds, from benzene to large polycyclic aromatic hydrocarbons (PAHs), are central building blocks of modern functional materials. Their delocalized π -electron systems give chemical stability, strong light absorption and emission, efficient charge transport and a strong tendency to self-assemble. This mini review traces the progression from classical aromatics (benzene, naphthalene, anthracene, pyrene) to heteroatom-engineered PAHs, with emphasis on boron–nitrogen (BN)-doped and boron–oxygen (BO)-fused frameworks. We summarize the main molecular engineering strategies — π -extension, ring fusion, heteroatom substitution, donor–acceptor design, multiple resonance (MR) architectures and supramolecular control and relate each to its effect on frontier orbital energies, photophysics, packing and stability. Representative applications in organic light-emitting diodes (OLEDs) and in fluorescent, chemical, gas and biological sensing are then discussed. Finally, we outline the remaining challenges, including synthetic complexity, aggregation-caused quenching, operational stability and scalability, and the directions most likely to shape next-generation aromatic materials.

Keywords: aromatic compounds; polycyclic aromatic hydrocarbons; heteroatom doping; BN-doped PAHs; multiple resonance; TADF; OLEDs; fluorescent sensors; structure–property relationships

1. Introduction

Aromatic compounds and PAHs are among the most important classes of organic molecules in chemistry and materials science. Since the discovery of benzene and the development of aromaticity theory, aromatic systems have driven advances in pharmaceuticals, dyes, polymers, catalysts and electronic materials [1,2]. Fused systems such as naphthalene, anthracene and pyrene attract particular attention for their extended π -conjugation, distinctive photophysics, thermal stability and tunable electronic properties [3,4]. These features make them candidates for optoelectronics, sensing, biomedical imaging and energy storage [5,6].

The growth of organic electronics has sharpened this interest. Delocalized π -systems support efficient charge transport, strong absorption, fluorescence and molecular self-assembly. These properties underpin OLEDs, organic field-effect transistors (OFETs), organic solar cells (OSCs), fluorescent sensors and photonic materials [7–9]. Pyrene- and anthracene-based compounds stand out as fluorescent and semiconducting materials, while benzene and naphthalene derivatives remain basic building blocks for industrial and functional materials [3].

A major recent advance is the incorporation of heteroatoms boron, nitrogen, oxygen, sulfur and phosphorus into polycyclic frameworks. Heteroatom engineering tunes frontier orbitals, charge distribution, aromatic stabilization and excited-state behavior [1,2,4]. BN-doped and BO-fused PAHs in particular deliver narrowband emission, high fluorescence quantum yields and improved thermal and chemical stability [10,11]. Figure 1 summarizes this progression from benzene to heteroatom-doped PAHs and the applications it enables.

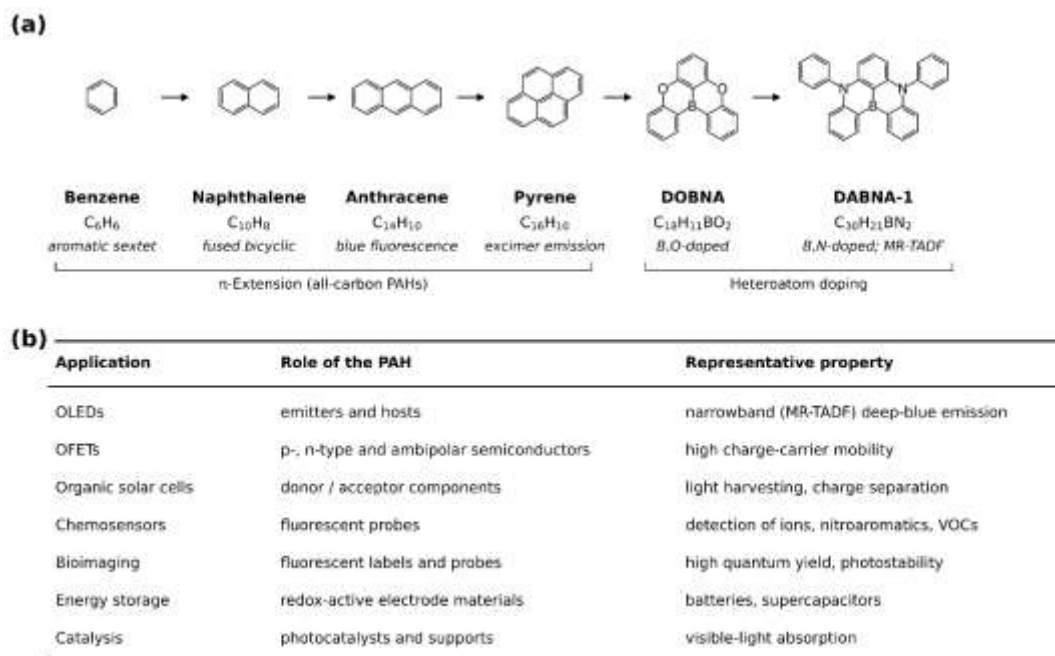


Figure 1. (a) Evolution of aromatic compounds from benzene through all-carbon PAHs to heteroatom-doped frameworks (DOBNA, DABNA-1). (b) Main applications of PAHs and the role each plays.

This mini review summarizes recent developments in aromatic and polycyclic aromatic compounds, focusing on structure–property relationships. Section 2 introduces classical aromatics and PAHs; Section 3 covers heteroatom engineering; Section 4 links molecular design to electronic, supramolecular and stability properties; Section 5 treats photophysics; Section 6 discusses OLED and sensing applications; and Section 7 outlines challenges and future perspectives.

2. From Benzene to Polycyclic Aromatic Hydrocarbons

2.1 Classical Aromatic Compounds

Benzene, naphthalene, anthracene and pyrene are the fundamental building blocks of aromatic chemistry. Each step along this series extends π -conjugation and changes the balance between stability, reactivity and optical activity (Table 1).

Benzene is the prototype aromatic hydrocarbon. Its planar ring and delocalized π -cloud give exceptional thermodynamic stability while allowing a wide range of substitution reactions. Benzene motifs appear throughout pharmaceuticals, agrochemicals, polymers and organic electronic materials, and benzene derivatives are key precursors to larger conjugated systems.

Naphthalene, with two fused rings, shows stronger π -conjugation and better electronic communication than benzene. Its rigid fused structure supports photostability and charge transport. Naphthalene derivatives are used in dyes, fluorescent probes, organic semiconductors, supramolecular assemblies and medicinal chemistry.

Anthracene, a linearly fused three-ring system, is notable for strong fluorescence, efficient charge transport and photoresponsive behavior. Its extended conjugation enables exciton migration and light harvesting, and its planarity supports strong solid-state π – π interactions. Anthracene derivatives are widely used in OLEDs, photoconductors, scintillators and fluorescence imaging [12].



Pyrene combines strong fluorescence, a long excited-state lifetime and excellent photostability. Its signature property is excimer formation through intermolecular π - π stacking. Pyrene derivatives therefore serve as fluorescent probes, bioimaging agents, OLED materials and OFET semiconductors with good charge-carrier mobility and self-assembly [7].

Table 1. Classical aromatics and representative PAHs: structural features, key properties and applications.

Compound / system	Structural feature	Key properties	Major applications
Benzene	Single aromatic ring	High stability; versatile substitution chemistry	Polymers, pharmaceuticals, precursors
Naphthalene	Two fused rings	Enhanced conjugation; photostability	Dyes, sensors, semiconductors
Anthracene	Three linearly fused rings	Blue fluorescence; charge transport	OLEDs, scintillators, imaging
Pyrene	Four fused rings, compact	Excimer emission; high quantum yield	Sensors, OFETs, bioimaging
Perylene	Five fused rings	High electron affinity; strong absorption	Solar cells, sensors
Coronene	Large disc-shaped core	Strong π -stacking; high conductivity	Energy devices, discotic materials

2.2 Polycyclic Aromatic Hydrocarbons

PAHs are fused systems of several benzene rings arranged in linear, angular or clustered topologies. Their electronic properties depend on the size of the conjugated core, its topology and the substitution pattern. Adding fused rings generally increases delocalization, narrows the HOMO–LUMO gap and raises charge-carrier mobility [3].

Linear acenes (anthracene, tetracene, pentacene) transport charge efficiently and have been widely used in OFETs and photovoltaics. Larger acenes, however, suffer from limited chemical stability and photooxidation [4]. This trade-off has motivated structurally modified PAHs that retain performance while improving stability.

Perylene, coronene and related extended PAHs show strong fluorescence, high absorption coefficients and efficient exciton transport. Their rigid planar cores promote ordered packing and charge migration in the solid state, making them active materials in OLEDs, OFETs, OSCs and photodetectors [3,13]. Their strong, environment-sensitive fluorescence also suits them to chemosensors for metal ions, explosives, volatile organic compounds (VOCs) and biomolecules, and to cellular imaging and photodynamic therapy [6]. Integration of PAHs into porous organic frameworks and carbon-rich nanostructures further extends their use to batteries, supercapacitors and photocatalysis [5,14].

3. Heteroatom Engineering of Aromatic Frameworks

Replacing carbon with B, N, O, S, P or Si is one of the most effective ways to tune an aromatic framework. The effect depends on the heteroatom's electronegativity, size, donor or acceptor character and orbital overlap with the π -system. As a rule, electron-deficient boron lowers the LUMO and favors electron transport, whereas electron-

rich nitrogen and sulfur raise the HOMO and favor hole transport [1,2]. Compared with all-carbon PAHs, heteroatom-modified systems often show higher fluorescence efficiency, better charge transport, greater thermal stability and narrower emission [2,4]. Figure 2 compares these effects across an isostructural series.

X	Structure	Electronic effect	Key properties	Applications
C (reference)		all-carbon parent; sp ³ C3 bridge	wide gap; blue emission; rigid	blue OLED hosts/emitters
N		π -donor (lone pair in π -system); HOMO raised	hole transport; high triplet energy; H-bonding (N-H)	OLED hosts; hole-transport layers; TADF donors
O		weaker π -donor than N; σ -withdrawing	high triplet energy; wide gap	OLED hosts; RTP and TADF materials
S		polarizable; heavy-atom effect (enhanced SOC)	S-S contacts; charge mobility; faster ISC	OPVs (e.g. BTBT); RTP
B		vacant p _z orbital; π -acceptor; LUMO lowered	electron transport; Lewis acidity; MR effect with N or O	anion (F ⁻ , CN ⁻) sensors; n-type and MR TADF emitters
P		σ^2 - π^* hyperconjugation; LUMO lowered; P-oxidation tunes	electron transport; thermal stability; flame retardancy	OLED electron-transport materials; sensors

All compounds share the dibenzo-fused five-membered (fluorene-type) framework, so differences arise from the bridging atom X.
Abbreviations: SOC, spin-orbit coupling; ISC, intersystem crossing; RTP, room-temperature phosphorescence; MR, multiple resonance.

Figure 2. Influence of the bridging heteroatom (X = C, N, O, S, B, P) on electronic effects, key properties and applications, compared across an isostructural series of dibenzo-fused five-membered rings (fluorene type). SOC, spin-orbit coupling; ISC, intersystem crossing; RTP, room-temperature phosphorescence; MR, multiple resonance.

3.1 Boron–Nitrogen (BN)-Doped PAHs

The B–N unit is isoelectronic and isostructural with C=C, so it can replace a carbon–carbon bond without disrupting the aromatic framework [15]. The polarity of the B–N bond, however, introduces electronic features that all-carbon systems cannot offer. BN doping regulates frontier orbital energies, electron density distribution and molecular packing [15].

The most important outcome is the BN-based multiple resonance (MR) emitter. Rigid frameworks with atom-localized frontier orbitals suppress vibrational relaxation and spectral broadening. The result is narrowband, high-color-purity emission with high fluorescence efficiency, especially valuable for deep-blue OLEDs [10,16,17]. BN units can also improve charge transport, exciton management and operational stability.

3.2 Boron–Oxygen (BO)-Fused PAHs

BO-fused PAHs combine electron-deficient boron centers with oxygen donors in a rigid fused core. They show strong fluorescence, excellent thermal stability and unusual excited-state behavior, including delayed fluorescence, room-temperature phosphorescence (RTP) and ultralong phosphorescence [11,18]. BO units also influence aromaticity, planarity and π – π interactions, and so affect charge transport and solid-state emission. Some BO-fused systems behave as promising n-type semiconductors.

3.3 Nitrogen-, Sulfur-, Oxygen- and Phosphorus-Containing Systems

Nitrogen incorporation alters electron density and strengthens intermolecular interactions, including hydrogen bonding and metal coordination. Azaacenes, carbazoles, quinolines, indoles and indolizines are widely used in semiconductors, electroluminescent materials and fluorescent probes [4]. Indole- and indolizine-fused systems have recently emerged as semiconductor platforms with tunable gaps and good mobility.



Sulfur-containing systems such as thiophenes and benzothiophenes benefit from sulfur's high polarizability, which promotes π - π stacking, $S \cdots S$ contacts and good film formation. They dominate conductive polymers, OFETs and organic photovoltaics [7]. Oxygen-containing systems, including furans and oxygen-fused PAHs, offer strong fluorescence and hydrogen-bonding ability for sensing and bioimaging. Phosphorus introduces distinctive electronic and coordination properties and often improves thermal stability, flame retardancy and electron transport, with uses in catalysis and luminescent materials [1].

Heteroatoms also strengthen spin-orbit coupling, promoting intersystem crossing and triplet formation. This is why heteroatom-modified aromatics frequently display thermally activated delayed fluorescence (TADF) and RTP [18,19]. Table 2 summarizes the main effects.

Table 2. Heteroatoms in aromatic frameworks and their functional consequences.

Heteroatom / system	Electronic effect	Resulting property	Major applications
Boron; BN-doped PAHs	Electron-deficient (vacant p orbital); localized frontier orbitals	Narrowband MR emission; high color purity	Deep-blue OLEDs, displays
B,O; BO-fused PAHs	Lowered LUMO; rigid fused core	Delayed fluorescence; ultralong phosphorescence	Luminescent devices, imaging
Nitrogen	π -donor; raises HOMO; polarity	Hole transport; environmental stability	OFETs, OLED hosts, sensors
Sulfur	High polarizability; heavy-atom effect	High mobility; faster ISC; RTP	OFETs, organic photovoltaics
Oxygen	Lone-pair interaction; H- bonding	Fluorescence tuning; high triplet energy	Sensors, bioimaging, TADF hosts
Phosphorus	$\sigma^*-\pi^*$ hyperconjugation; lowers LUMO	Electron transport; thermal stability	Electron-transport layers, catalysis

4. Molecular Engineering and Structure–Property Relationships

Rational molecular design lets chemists set energy levels, emission color, charge transport, packing and stability almost independently. The main strategies are summarized in Figure 3 and Table 3.

Strategy	Approach	Representative example	Effect on properties
Structural	n-Extension	 pentacene	longer conjugation; narrower HOMO–LUMO gap
	Planarization	 9,9-dimethylfluorene	bridged triphenyl; rigid, planar, higher Φ_p
	Steric modulation	 TIPS-pentacene	bulky groups: solubility, stability, 2D π -stacking
Heteroatom	B,N substitution	 dibenzo-1,4-azaborine	isoelectronic B–N for C=C; tunable gap
	B,O substitution	 dibenzo-1,4-oxaborine	lowered LUMO; deep-blue emission
	S incorporation	 8TBT	S–S contacts: high hole mobility
	N incorporation	 carbazole	electron-rich donor; raised HOMO
Electronic	Donor–acceptor	 PXZ-TRZ	ICT; small ΔE_{ST} (TADF)
	Multiple resonance	 DABNA-1	atom-separated HOMO/LUMO; narrowband emission
	Energy-level tuning	EWG (F, CN) / EDG (OMe, NR ₂)	shifts HOMO/LUMO and redox potentials
Supramolecular	Packing control	side chains, H-bonding, halogen bonding	herringbone vs. brick-wall; charge transport
	Aggregation control	 tetraphenylethylene	aggregation-induced emission; suppresses ACQ
Computational	In silico design	DFT / TD-DFT; machine-learning screening	predicts gaps, ΔE_{ST} , transport; guides synthesis
Tailored properties:		tunable energy levels, high Φ_p , narrowband emission, efficient charge transport, stability	
Applications:		OLEDs, OFETs, organic solar cells, sensors, bioimaging, energy storage, photocatalysis	

Figure 3. Molecular engineering strategies for aromatic materials — structural, heteroatom, electronic, supramolecular and computational — with representative examples and their effects on properties.

4.1 Electronic Structure: π -Extension, Ring Fusion and Donor–Acceptor Design

The HOMO–LUMO gap governs absorption wavelength, emission color, conductivity and redox behavior. Extending conjugation through ring fusion lowers this gap, red-shifts absorption and emission, and raises carrier mobility [3]. Fusion also rigidifies and planarizes the core, suppressing non-radiative loss. Topology matters as well: linear acenes have smaller gaps and higher mobility than angular or non-planar analogues, but very large planar cores risk aggregation-caused quenching (ACQ) and poor solubility [20].

Donor–acceptor (D–A) design places electron-rich and electron-deficient units in one conjugated framework, enabling intramolecular charge transfer (ICT). Adjusting donor strength, acceptor strength and bridge length tunes the optical gap, broadens absorption and controls the singlet–triplet gap (ΔE_{ST}). D–A systems underpin TADF emitters, solar-cell materials, solvatochromic sensors and photocatalysts [9,21].

4.2 Multiple Resonance Architectures

MR emitters place electron-donating and electron-accepting atoms in alternating positions of a rigid polycyclic core. The HOMO and LUMO localize on different atoms with minimal overlap, while the rigid core limits structural relaxation in the excited state. This combination gives ultranarrow emission, high quantum efficiency and low energy loss. BN-doped MR emitters such as DABNA-1 have set benchmarks for deep-blue OLEDs [10,16,17].



4.3 Supramolecular Organization

Non-covalent interactions decide how molecules pack, and packing decides much of device performance. Close, ordered π - π stacking increases intermolecular electronic coupling, exciton migration and carrier mobility [7,13]. Excessive aggregation, however, causes fluorescence quenching and trap states. Bulky substituents, twisted geometries and side-chain design are therefore used to balance coupling against emission.

Hydrogen bonding, dipole-dipole and donor-acceptor interactions provide further control. Heteroatom-containing aromatics can form hydrogen-bonded assemblies with improved rigidity and stability. Pyrene, perylene and discotic aromatics self-assemble into nanofibers, nanosheets, vesicles and columnar stacks. These structures support charge transport in electronics, exciton migration in photovoltaics and drug encapsulation in biomedicine [13]. Assemblies that respond to temperature, pH, solvent, light or mechanical force are being developed for sensing, data storage and anti-counterfeiting.

4.4 Stability Enhancement

Aromatic delocalization confers intrinsic stability, but large acenes such as tetracene and pentacene remain prone to photooxidation and degradation [4]. Four strategies address this. Ring fusion and rigidification suppress excited-state distortion and photochemical damage. Heteroatom engineering, notably BN and BO fusion, stabilizes frontier orbitals and excited states. Steric protection with bulky groups shields reactive sites and prevents uncontrolled aggregation. Finally, encapsulation and protective coatings guard against oxygen and moisture. Fused, rigid architectures also raise glass-transition and decomposition temperatures, improving device reliability.

4.5 Computational Design

Density functional theory (DFT), time-dependent DFT (TD-DFT), electrostatic potential mapping and molecular dynamics are now standard tools. They predict frontier orbital energies, Δ EST, aromaticity, packing energies and degradation pathways (e.g., bond dissociation energies and oxidation potentials) before synthesis [22,23]. Combined with X-ray crystallography, they guide the rational design of new aromatic materials.

Table 3. Molecular engineering strategies and their structure-property-application outcomes.

Strategy	Structural change	Resulting property	Application area
π -Extension	Longer conjugation	Smaller HOMO-LUMO gap; red-shifted absorption	Semiconductors, photodetectors
Ring fusion / planarization	Greater rigidity and planarity	Better charge transport; higher fluorescence quantum yield	OFETs, OLEDs
BN substitution	Polarized π -system; localized orbitals	Narrowband MR emission	Deep-blue OLEDs
BO fusion	Rigid B,O-embedded core	Delayed fluorescence; persistent luminescence	OLEDs, imaging
Donor-acceptor design	Intramolecular charge transfer	Tunable gap; small Δ EST	TADF-OLEDs, solar cells
Supramolecular control	Ordered π -stacking; H-bonding	Higher mobility; exciton migration	Electronic devices
Steric modulation	Bulky or twisted substituents	Less ACQ; better stability	Sensors, solid-state emitters

5. Photophysical Properties

The optical behavior of aromatic compounds originates in their delocalized π -systems and is shaped by conjugation length, rigidity, heteroatom content and intermolecular interactions. Figure 4 summarizes the main excited-state pathways, and Table 4 relates them to applications.

Absorption and fluorescence. Aromatics absorb strongly in the UV–visible region through π – π^* transitions [22]. Extending conjugation red-shifts absorption and raises molar absorption coefficients, so perylene and coronene cover the spectrum more broadly than benzene or naphthalene. Fluorescence arises from radiative $S_1 \rightarrow S_0$ decay. Rigid, planar cores restrict molecular motion and suppress non-radiative decay, which is why anthracene and pyrene derivatives combine high quantum yields with good photostability.

Excimer emission. Pyrene forms excited-state dimers (excimers) when two molecules stack face to face at about 3.4 Å. Excimer emission is broad and red-shifted (about 460–480 nm) relative to the structured monomer band (370–400 nm). Because the excimer-to-monomer ratio depends on distance and environment, pyrene is a sensitive ratiometric probe of ions, biomolecules, viscosity and polarity.

Phosphorescence and delayed fluorescence. Purely organic aromatics usually phosphoresce weakly because intersystem crossing (ISC) is slow. Heteroatoms (B, N, O, S) enhance spin–orbit coupling and enable RTP and ultralong phosphorescence [18,19]. In TADF emitters, a small ΔE_{ST} allows reverse intersystem crossing (RISC) from T_1 to S_1 , so triplet excitons are harvested as delayed fluorescence [9,21].

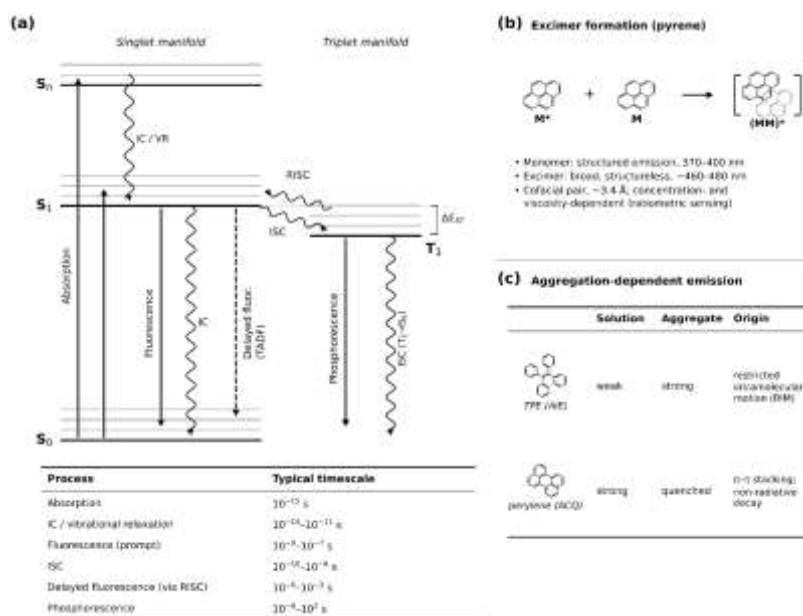


Figure 4. Photophysical processes in aromatic materials. (a) Jablonski diagram showing fluorescence, ISC, phosphorescence and TADF via RISC, with typical timescales. (b) Pyrene excimer formation. (c) Aggregation-dependent emission: AIE (tetraphenylethylene) versus ACQ (perylene).

Aggregation effects. Strong stacking in planar aromatics often causes ACQ. Aggregation-induced emission (AIE) luminogens such as tetraphenylethylene behave oppositely: restricted intramolecular motion in the aggregate



blocks non-radiative decay and switches emission on [20]. Steric engineering and AIE design are the main tools for bright solid-state emission.

Charge-transfer emission. ICT in D–A systems produces solvatochromism, broad absorption, dual emission and environment-sensitive fluorescence, all exploited in sensors, bioimaging and photovoltaics.

Table 4. Photophysical processes in aromatic systems.

Process	Mechanism	Key feature	Representative systems	Applications
Fluorescence	$S_1 \rightarrow S_0$ radiative decay	Fast (ns) emission	Anthracene, pyrene	OLEDs, probes
Excimer emission	Excited-state π -stacked dimer	Ratiometric, environment-sensitive	Pyrene	Sensors, biosensing
Phosphorescence / RTP	$T_1 \rightarrow S_0$ via enhanced ISC	Long-lived emission	BO-fused, S-containing PAHs	Imaging, anti-counterfeiting
TADF	RISC across small ΔE_{ST}	Harvests triplets	D–A and MR-TADF emitters	OLEDs
MR emission	Atom-separated HOMO/LUMO in rigid core	Narrow FWHM; high color purity	BN-doped PAHs	Displays
AIE	Restricted intramolecular motion	Bright solid-state emission	Tetraphenylethylene	Bioimaging, sensors

6. Applications

6.1 Organic Light-Emitting Diodes

OLEDs are the most successful commercial use of aromatic materials, offering high brightness, low power consumption, wide viewing angles and mechanical flexibility [12]. Device performance depends directly on the emitter's quantum yield, charge transport, color purity and stability.

Anthracene and pyrene fluorophores were early workhorses. Anthracene's wide gap and efficient singlet emission suit blue OLEDs, while pyrene offers high quantum yields and good charge transport for emissive and transport layers. Deep-blue emission nevertheless remains the hardest target: blue emitters need high excitation energies yet must stay efficient and stable, and conventional fluorophores suffer from broad spectra, efficiency roll-off and short lifetimes [12].

Three developments have changed this picture. First, BN-doped MR emitters give deep-blue emission with very small full width at half maximum (FWHM), high quantum yields and high external quantum efficiencies (EQEs), meeting ultra-high-definition display standards [10,16]. Second, BO-fused PAHs combine rigid cores, narrow emission and excellent thermal stability, and several deliver efficient deep-blue electroluminescence [11]. Third, TADF emitters harvest both singlet and triplet excitons through RISC, allowing internal quantum efficiencies approaching 100% when ΔE_{ST} is minimized [9,21,24]. Combining TADF with MR design (MR-TADF) now yields narrowband emitters with low roll-off and outstanding electroluminescence [17].

6.2 Sensors and Detection Systems

Tunable electronic structure, strong fluorescence and specific molecular interactions make aromatic compounds versatile sensing platforms. The main signaling mechanisms — photoinduced electron transfer (PET), ICT, Förster resonance energy transfer (FRET), excimer/monomer switching, intercalation and chemiresistive response — are summarized in Figure 5 [6].

Mechanism	Representative probe	Analyte	Signal	Application
Photoinduced electron transfer (PET)	 anthracene-aza-crown (fluorophore-spacer-receptor)	K^+ , Na^+ , H^+	turn-on; binding blocks N lone-pair PET	clinical electrolytes; pH sensing
Fluorescence quenching by electron-poor analytes	 analyte: TNT (with pyrene or PAH films)	nitroaromatic explosives	turn-off; electron transfer $PAH^* \rightarrow$ analyte	security; vapour detection
Excimer / monomer ratio	 1-pyrenebutyric acid	O_2 , metal ions, DNA, proteins	ratiometric: I_e/I_m (~480 vs 375-395 nm)	biosensing; O_2 sensing
Intramolecular charge transfer (ICT)	 dansylamide	polarity, proteins, Zn^{2+}	λ_{em} shift with local polarity or binding	protein labelling; bioimaging
Intercalation	 ethidium	double-stranded DNA / RNA	~20-fold emission increase on intercalation	gel staining; diagnostics
FRET	donor/acceptor pair (e.g. pyrene/perylen)	nucleic acids, proteases	distance-dependent energy transfer (1-10 nm)	molecular beacons; assays
Chemiresistive / OPET response	PAH or thiophene-fused semiconductor film	NH_3 , NO_2 , H_2S , VOCs	change in current, mobility or V_{th}	gas and environmental monitoring

I_e/I_m , excimer-to-monomer intensity ratio; V_{th} , threshold voltage; FRET, Förster resonance energy transfer.

Figure 5. Sensing mechanisms of aromatic fluorophores and semiconductors, with representative probes, target analytes, signal outputs and applications. I_e/I_m , excimer-to-monomer intensity ratio; V_{th} , threshold voltage.

Fluorescent sensors. Analytes are detected through changes in emission intensity, wavelength, lifetime or excimer ratio. Probes bearing N, O, S or P donor sites coordinate metal ions such as Hg^{2+} , Cu^{2+} , Fe^{3+} , Zn^{2+} , Pb^{2+} and Cd^{2+} , producing turn-on, turn-off or ratiometric responses for water-quality and biomedical analysis [6,20]. Electron-poor nitroaromatic explosives (TNT, DNT, picric acid) quench electron-rich pyrene, anthracene and perylene fluorophores by PET, enabling fast, portable security screening [20].

Chemical and gas sensors. Pyrene-containing polymers and conjugated frameworks respond to VOCs such as benzene, toluene, xylene, acetone and formaldehyde through changes in emission, excimer formation or conductivity. Aromatic semiconductors and thiophene-fused films detect NH_3 , NO_2 , CO and H_2S as changes in current or threshold voltage [25]. Related probes monitor pesticides and industrial pollutants in water, soil and air.

Biosensors and bioimaging. Functionalized aromatic fluorophores recognize proteins, enzymes, nucleic acids, carbohydrates and amino acids. Intercalating or groove-binding probes report on DNA and RNA for mutation detection and pathogen identification [6]. Combining aromatic fluorophores with nanomaterials, polymers, AIE



luminogens and supramolecular assemblies has lowered detection limits and improved selectivity and biocompatibility [6]. Self-assembled aromatic nanostructures are also being explored for drug delivery and theranostics.

6.3 Energy and Catalysis

Extended aromatic systems with high conductivity and stable redox behavior are under study as electrode materials for batteries and supercapacitors, as hydrogen-storage media and as visible-light photocatalysts. Their integration into porous organic frameworks and carbon-rich nanostructures is a growing route to sustainable energy storage and conversion [5,14].

7. Challenges and Future Perspectives

Despite rapid progress, several obstacles still limit practical use of functional aromatic materials:

- **Synthetic complexity and scalability.** Multistep syntheses, difficult purification and low yields of large or heteroatom-doped PAHs hinder commercialization.
- **Solid-state quenching.** Controlling aggregation while keeping high luminescence efficiency in films remains difficult.
- **Operational stability.** Photooxidation, moisture sensitivity and degradation under device operation, especially for deep-blue emitters, shorten lifetimes.
- **Environmental and health concerns.** The toxicity of some PAHs calls for careful design, handling and disposal [26].

Several directions look most promising. New heteroatom combinations and MR-TADF architectures should push color purity and efficiency further. Stimuli-responsive and bioinspired aromatic systems may open uses in smart materials, data security and theranostics. Greener, scalable syntheses and solution-processable, air-stable materials are needed for printable and flexible electronics. Finally, computational screening, including machine-learning approaches, can shorten the design–synthesis–testing cycle [23].

8. Conclusions

Aromatic compounds, from benzene to extended and heteroatom-doped PAHs, offer an unusually versatile platform for tuning electronic, optical, photophysical and supramolecular properties. π -Extension, ring fusion, heteroatom incorporation, donor–acceptor design and supramolecular control now allow precise adjustment of energy levels, charge transport, emission color, efficiency and stability. BN-doped and BO-fused frameworks have been especially important, giving access to narrowband MR emission, TADF and room-temperature phosphorescence. These advances have produced efficient OLEDs, OFETs and photovoltaic materials, as well as sensitive probes for metal ions, explosives, VOCs, gases and biomolecules. Future progress will depend on combining several functions in one molecular platform while meeting the demands of sustainable synthesis, scalable manufacturing and long-term stability.

Conflicts of Interest: The authors declare no conflicts of interest.

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