

Recent advances in organic fluorescent and hybrid chemosensors for Lead ion detection in environmental applications

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ABSTRACT

Lead ion (Pb^{2+}) contamination poses a serious threat to both environmental and human health due to its high toxicity, even at trace levels. Consequently, the demand for ultrasensitive, selective, and practical detection methods has become increasingly critical for effective monitoring and remediation efforts. Among the available techniques, fluorescent chemosensors stand out for their rapid, sensitive, and often visible responses to Pb^{2+} , enabling on-site and real-time detection. The organic small molecular fluorescent probes offer significant advantages for sensing applications, including structural tunability, ease of functionalization, large Stokes shift, photostable, tunable optical properties, high sensitivity and selectivity. This review presents a comprehensive overview of recent developments (2020–2025) in organic fluorescent and colorimetric chemosensors for Pb^{2+} detection, emphasizing both chemical innovations and practical applications. This review systematically explores various modern chemosensor materials such as rhodamine, triazole, peptide-based derivatives, and a wide range of Schiff-base compounds including imines, azines, and azo derivatives. It also highlights the emerging role of metal-organic frameworks (MOFs), covalent organic frameworks (COFs), and hybrid architectures in enhancing sensitivity and selectivity toward lead ions. In addition, this review delves into the fundamental principles of fluorescence-based Pb^{2+} sensing, outlining key design strategies, the influence of functional groups, sensing

Abbreviations: COF, Covalent organic framework; MOF, Metal organic framework; Pb, Lead; IQ, Intelligence quotient; WHO, World Health Organization; USEPA, U.S. Environmental Protection Agency; $\mu\text{g/dL}$, microgram per decilitre; AAS, Atomic absorption spectroscopy; ICP-MS, Inductively coupled plasma mass spectrometry; B-H, Benesi-Hildebrand; mg/L , Milligram per litre; Ppb, Parts per billion; SDG, Sustainable Development Goals; N, Nitrogen; O, Oxygen; S, Sulphur; PET, Photoinduced Electron Transfer; ESIPT, Excited-State Intramolecular Proton Transfer; ICT, Intramolecular charge transfer; CHEF, Chelation-Enhanced Fluorescence; Cu, Copper; RSD, Relative standard deviation; %, Percentage; Hg, Mercury; Cd, Cadmium; EtOH, Ethanol; v/v, Volume/volume; EDTA, Ethylenediaminetetraacetic acid; DFT, Density functional theory; LUMO, Lowest unoccupied molecular orbital; HOMO, Highest occupied molecular orbital; DNA, Deoxyribonucleic acid; Kcal mol^{-1} , Kilocalories per mole; pH, Power of hydrogen; λ_{ex} , Excitation wavelength; λ_{em} , Emission wavelength; HEPES, 4-(2-hydroxyethyl)-1-piperazineethanesulfonic acid; λ_{max} , maximum wavelength; TDDFT, Time dependent density functional theory; μM , Micromolar; LOD, Limit of detection; Co, Cobalt; UV-Vis, Ultraviolet visible; REHBA, Rhodamine hydrazide and 2,3,4-trihydroxybenzaldehyde; HepG2, human liver cancer cell line; LCCT, Ligand-to-Cluster Charge Transfer; ESI-MS, Electrospray ionization mass spectrometry; RPU, Rhodamine-phenylurea; Zn, Zinc; Mg, Magnesium; $^1\text{H-NMR}$, proton nuclear magnetic resonance; K_{SV} , Stern-Volmer constant; K_{a} , Acid dissociation constant; CH_3CN , Acetonitrile; CuAAC, Cu(I)-catalyzed alkyne-azide cycloaddition; Mn, Manganese; CPT, Cresolphthalein; HSAB, Hard and soft acid-based theory; FTIR, Fourier-transform infrared spectroscopy; DMSO, Dimethyl sulfoxide; eV, electron volt; $^{\circ}\text{C}$, degree centigrade; CH_3OH , Methanol; *E. coli*, *Escherichia coli*; DQS, Dimeric quinoline Schiff base; AIE, Aggregation induced emission; v/v, volume/volume; QMC, 2-chloro-3-formylquinoline and morpholine; nM, Nanomolar; LMCT, Ligand-to-metal charge transfer; QTAIM, Quantum Theory of Atoms in Molecules; Cr, Chromium; *Equiv.*, Equivalent; NIR, Near infrared region; FL, Fluorescence; *C. elegans*, *Caenorhabditis elegans*; LC-MS, Liquid chromatography-mass spectrometry; In, Indium; SPPS, Solid-phase peptide synthesis; Gly-Ser-Met-COOH, Glycyl-L-seryl-L-methionine-carboxylic acids; HeLa, Human cell line derived from Henrietta Lacks; Cys, Cysteine; HPLC, High performance liquid chromatography; NaCl, Sodium chloride; mM, millimolar; DMF, Dimethyl formamide; K, Potassium; PVC, Polyvinyl chloride; NPOE, 2-Nitrophenyl octyl ether; Ca, Calcium; Ag, Silver; XRD, X-ray Diffraction; BET, Brunauer, Emmett and Teller; SEM, Scanning electron microscopy; ICP-OES, Inductively coupled plasma optical emission spectroscopy; TGA, Thermogravimetric analysis; DSC, Differential scanning calorimetry; PL, Photoluminescence; TNP, 2,4,6-trinitrophenol; NIP, Non-imprinted polymers; S-V, Stern-Volmer; EBT, Eriochrome Black T; BTB, Bromothymol Blue.

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mechanisms and potential real-world applications. This work aims to serve as a valuable guide for researchers developing next-generation organic fluorescent probes for efficient and selective lead ion detection.

1. Introduction

Lead (Pb) is recognized as the second most toxic heavy metal and is non-biodegradable, posing serious risks to both human health and the environment [1–3]. Even at very low concentrations, Pb exposure particularly in children can result in irreversible neurological and physiological damage, including impaired cognitive development, stunted physical growth, and developmental delays [4]. Other reported health effects encompass anemia, reduced intelligence quotient (IQ), memory deficits, irritability, muscular paralysis, renal dysfunction, and long-term neurological disorders. Despite these well-established toxicities [5], Pb remains widely used in modern industries, including insulation materials, protective coatings, electronic components, paints, and storage batteries [6,7]. Because of its continued use, there is an urgent need for extremely sensitive and selective detection of Pb^{2+} at levels lower than the U.S. Environmental Protection Agency (USEPA) and World Health Organization (WHO) guidelines, which are 10 ppb (48 nM) and 16 ppb (77 nM) for drinking water, respectively [8,9].

In the human body, Pb is widely distributed to sensitive organs, including the brain, liver, kidneys, and bones, where its long-term accumulation primarily occurs in bones and teeth. Normally, Pb concentrations in blood are expected to remain at approximately 10 $\mu\text{g}/\text{dL}$ in adults and 1.4 $\mu\text{g}/\text{dL}$ in children; values above these levels indicate harmful exposure [10,11]. This bioaccumulation, coupled with slow excretion, makes Pb a persistent public health hazard, necessitating constant monitoring in environmental and biological systems. The traditional detection methods such as atomic absorption spectrometry (AAS), inductively coupled plasma mass spectrometry (ICP-MS), and inductively coupled plasma atomic emission spectroscopy (ICP-AES) deliver excellent sensitivity and selectivity, with detection limits often reaching 0.2–2.5 $\mu\text{g}/\text{L}$ [12–14]. These techniques are considered gold standards for precise quantification in both environmental and clinical samples. However, their practical application is curtailed by several limitations, including high instrument costs, lack of portability, complicated analytical procedures, extended analysis times, and the requirement for highly skilled operators. Consequently, there is a pressing demand for alternative methods that are not only cost-effective and user-friendly but also suitable for rapid, real-time, or field-deployable Pb^{2+} detection.

To overcome these challenges, simpler approaches such as colorimetric assays have been widely explored. Colorimetric detection is based on visible color changes resulting from interactions between Pb^{2+} and organic chromophores, chelating dyes, or nanomaterials [15–19]. In classical examples, complexes with dyes such as dithizone exhibit distinct absorption spectrum changes upon Pb^{2+} binding, producing easily perceivable color variations. Recent strategies frequently rely on functionalized nanoparticles (e.g., gold nanoparticles) [20], where Pb-induced aggregation or plasmon resonance shifts provide clear visual signals [17,18,21–23]. These assays are advantageous due to their operational simplicity, low cost, minimal instrumentation, and ability to produce immediate qualitative or semi-quantitative outputs. Furthermore, their compatibility with portable devices including smartphone imaging and machine-learning-based analysis opens possibilities for decentralized monitoring and emergency assessments. However, their moderate sensitivity, potential interference from coexisting ions, and occasional reliance on toxic reagents limit widespread adoption in complex real-world matrices [24,25].

On other hand, the fluorometric methods offer much higher sensitivity and selectivity [26]. These systems utilize the modulation of fluorescence emission intensity or wavelength upon Pb^{2+} binding with organic or hybrid probes. The fluorescence responses may manifest as

emission increases (“turn-on”), quenching/shifts (“turn-off”), or ratio-metric responses that allow self-calibration [24,27–33]. Classical examples include rhodamine-based probes, which undergo structural transformations leading to strong signal modulation. Incorporation of fluorophores into polymeric matrices, hydrogels, or nanocarrier systems further enhances signal amplification, reaching sub-ppb detection limits and enabling rapid quantitative analysis [34–36]. In contrast to colorimetric assays, fluorometric techniques provide not only fast response times but also strong quantitative reliability, making them highly competitive with conventional spectroscopic techniques. Moreover, their potential for integration into wearable, portable, and bioimaging platforms broadens their applicability from environmental sensing to biomedical diagnostics. However, challenges such as sensitivity to matrix interferences, competing metal ions, and the continuing requirement for optical instrumentation remain significant [37,38]. The need for sensitive and selective Pb^{2+} detection is underscored by the fact that its health hazards occur at concentrations as low as parts per billion (ppb). Reliable methods must therefore be capable of monitoring trace Pb^{2+} in diverse and complex environments without interference, while still being affordable and straightforward for practical deployment. In this context, colorimetric and fluorometric approaches have emerged as powerful alternatives to conventional techniques, offering the benefits of low cost, portability, rapid signal readout, and potential for real-time monitoring. Both strategies continue to evolve, with recent advancements focusing on refining probe design, improving selectivity, and enhancing detection performance under real-world conditions.

Although numerous review articles have summarized the broader principles of heavy metal ion detection using optical or electrochemical transduction approaches [39–44]. For instance, two report in 2021 described nanomaterial-based fluorescent sensors for lead ion detection [38,45]. However, to the best of our knowledge, no comprehensive review has yet highlighted organic fluorescent ligands specifically designed for selective Pb^{2+} sensing. The current work aims to fill this gap by presenting an in-depth discussion of recent advances in organic probe-based detection systems. Particular emphasis is placed on rhodamine-, triazole-, imine-, azine-, peptide-, metal organic framework (MOF)-, and covalent organic framework (COF)-based chemosensors. We further explore their sensing mechanisms, the design principles underlying selective signal responses, and the challenges that must be addressed to enable practical applications in environmental monitoring and biomedical analysis.

2. Mechanisms of organic-based fluorescent materials for Pb^{2+} ion sensing

In order to comprehend the fluorescence properties of various probes, it is essential to recognize systems may function through either specific host-guest interactions or selective chemical reaction pathways. The validation of their fluorescence behaviour requires an understanding of binding interactions, particularly within host-guest chemistry. These interactions are typically non-covalent and reversible, such systems are often designated as chemosensors. Notably, variations in fluorescence intensity and emission wavelength directly reflect recognition events between probe binding sites and target analytes. The rational design of fluorescent probes, particularly tailoring of the fluorophore component, is therefore critical to regulate fluorescence “switch-off/on” behaviour and enhance emission intensity. A typical fluorescent chemosensor is composed of three functional elements: (i) a fluorophore, responsible for light absorption and emission as well as signal transduction; (ii) a receptor unit (recognition site) that selectively binds analytes (example for Pb^{2+}); and (iii) a linker/spacer connecting

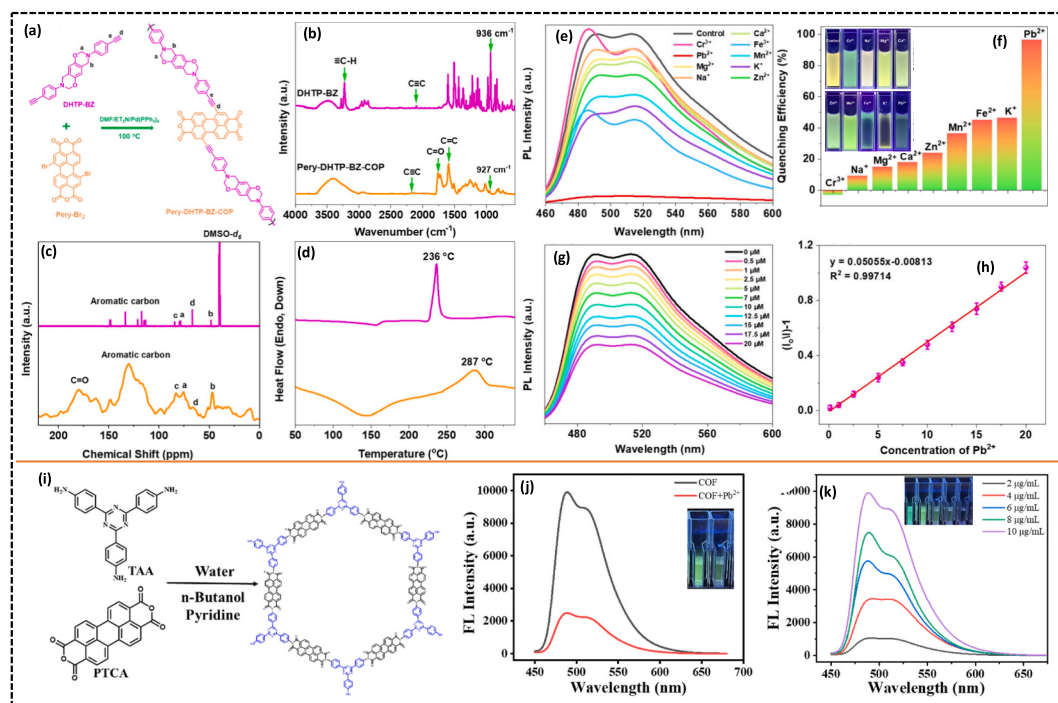


Fig. 20. (a) Synthetic route of Pery-DHTP-BZ-COP; (b) FT-IR; (c) ^{13}C NMR; and (d) DSC spectra of DHTP-BZ and Pery-DHTP-BZ-COP; (e) Photoluminescence spectra of Pery-DHTP-BZ-COP in the presence of different metal ions; (f) Corresponding quenching efficiencies (inset: UV images of Pery-DHTP-BZ-COP with various metal ions); (g) Fluorescence titration with increasing Pb^{2+} concentration; and (h) Linear correlation between PL intensity and Pb^{2+} concentration [154]; (i) Synthetic route of Polyimide COF (TTA-PTCA); (j) FL intensity of the TTA-PTCA at different concentrations (inset: corresponding images at varying concentrations); (k) Fluorescence intensity of the TTA-PTCA before and after addition of Pb^{2+} (inset: images showing the change upon Pb^{2+} addition) [155]. (Permission has taken from Reference no. [154,155]).

peak at $\sim 287^\circ\text{C}$, significantly higher than that of the DHTP-BZ monomer, which indicates hindered ring-opening polymerization in the rigid COP backbone and enhanced thermal stability of the material (Fig. 20d). The fluorescence behaviour of Pery-DHTP-BZ-COP in solution was examined by photoluminescence spectroscopy. The polymer displayed distinct solvent-dependent emission, with maximum intensity observed in methanol. Its electron-rich composition facilitated efficient charge transfer to electron-deficient analytes, enabling sensing applications. Under UV illumination, the bright yellow emission of the polymer was markedly quenched only in the presence of Pb^{2+} , while other metal ions produced negligible effects (Fig. 20e). The PL spectra and quenching efficiency analysis confirmed a strong interaction, with Pb^{2+} achieving nearly 97% quenching (Fig. 20e, f). The fluorescence titration revealed a systematic decrease in PL intensity with increasing Pb^{2+} concentration, yielding an excellent linear correlation (Fig. 20g, h). This response corresponded to a LOD as low as $0.5\ \mu\text{M}$, consistent with a PET-based quenching mechanism [154].

Yu et al. reported the synthesis of a luminescent polyimide covalent organic framework (Polyimide COF (TTA-PTCA)) by condensing 4,4',4''-(1,3,5-triazine-2,4,6-triyl) triphenylamine (TTA) with perylene-3,4,9,10-tetracarboxylic dianhydride (PTCA) under solvothermal conditions. The schematic design of the fluorescence/smartphone dual-mode sensing platform based on this COF is illustrated in (Fig. 20i). The structural characterization confirmed the successful formation of imide-linked framework, the FT-IR spectrum displayed characteristic C=O and C–N–C vibrations, while solid-state ^{13}C -NMR showed signals for carbonyl and aromatic carbons. The XRD analysis revealed distinct diffraction peaks, verifying the crystalline nature of the COF, and SEM/TEM images demonstrated a lamellar sheet-like morphology with a uniform pore structure. The BET analysis indicated supermicroporous/mesoporous features, providing a high surface area conducive to ion capture. The photoluminescence behaviour of the COF was studied in aqueous medium. Upon excitation at $436\ \text{nm}$, the COF exhibited a strong

emission band centered at $496\ \text{nm}$. Fig. 20j shows that fluorescence intensity increased systematically with COF concentration, particularly in the $0.001\text{--}0.01\ \text{mg/mL}$ range confirming tunable emission properties. In contrast, Fig. 20k highlights the quenching response to Pb^{2+} , where the emission at $496\ \text{nm}$ rapidly decreased within one minute, clearly visible even to the naked eye, reflecting the sensor's high responsiveness. The sensing performance was further examined by fluorescence titration, which revealed a progressive reduction in emission intensity with increasing Pb^{2+} concentration. The quenching was attributed to a synergistic mechanism involving FRET, PET, π - π stacking and dynamic quenching. The system exhibited a wide linear range from $0.1\ \text{nM}$ to $1\ \mu\text{M}$ with an ultralow LOD of $50\ \text{pM}$ (picomolar), surpassing the EPA threshold of $15\ \mu\text{g/L}$. In addition, smartphone-assisted RGB analysis enabled visual readouts, and machine learning models provided precise quantification. The COF sensor also showed excellent selectivity against competing metal ions, retained 94% of its fluorescence signal over 30 days, and remained reusable for at least five cycles. The swab-based sampling further demonstrated its practicality in field conditions, while recovery experiments in real water samples achieved 101–104%, consistent with ICP validation [155].

Similarly, Rene et al., synthesized fluorescent ion-imprinted polymers (IIPs) and characterized for the selective detection of Pb^{2+} using a functional monomer, ANQ-ST, which incorporates a chelating 5-amino-8-hydroxyquinoline moiety. The Pb^{2+} detection was carried out in a water-acetone mixture ($1:4\ \text{v/v}$), with fluorescence enhancement observed upon Pb^{2+} binding. The sensor demonstrated a LOD of $2.4\ \mu\text{g/L}$, significantly below international safety thresholds, such as the WHO standard of $10\ \mu\text{g/L}$. The UV-Vis spectroscopy and modeling confirmed a $1:2$ binding stoichiometry between Pb^{2+} and ANQ-ST under optimal conditions using a DMSO-MeOH solvent and a 0.42 metal/ligand ratio. The imprinting process enhanced specificity, as evidenced by higher fluorescence responses compared to non-imprinted polymers (NIPs). The competitive ion studies showed minimal interference from ions such

as Ag^+ , Na^+ , Ca^{2+} , Cd^{2+} , Co^{2+} , Cu^{2+} and Zn^{2+} , even at high concentrations. The calibration studies revealed high recovery rates (96–113%) for Pb^{2+} in spiked samples of tap water, mineral water, and seawater, highlighting the sensor's reliability for practical environmental monitoring. Furthermore, the sensor's robust performance across various pH levels and aqueous matrices demonstrated its broad applicability and high selectivity for Pb^{2+} [156].

11. Conclusion and outlooks

Over the past five years, remarkable progress has been made in the design of organic fluorescent and colorimetric chemosensors for Pb^{2+} detection, as supported by numerous reports in recent literature. These review efforts encompass a wide variety of molecular architectures, such as rhodamine derivatives, imine-based Schiff bases, triazole scaffolds, peptides, and azo/azine compounds, as well as extended porous architectures like MOFs and COFs. Initially, we examined the underlying mechanisms of organic-based fluorescent materials for Pb^{2+} ion sensing, which highlighted how structural flexibility, donor-acceptor modulation, and electronic transitions govern sensing behaviour. Building on this foundation, we first considered rhodamine-based fluorescent chemosensors, which continue to serve as a benchmark for Pb^{2+} sensing due to their well-defined spirolactam ring-opening mechanism. This mechanism allows excellent sensitivity and selectivity, particularly when combined with rational structural design strategies. Expanding beyond rhodamine systems, peptide-derived fluorescent probes emerged as a rapidly growing class. Their sequence-specific adaptability, defined coordination sites and tunable photophysical responses provide unique opportunities for biological applications, especially in complex cellular

environments. Schiff base-derived probes, benefiting from the versatile $\text{C}=\text{N}$ linkage, have demonstrated strong Pb^{2+} chelation, tunable photophysical transitions and flexibility in functionalization, enabling mechanisms such as ESIPT suppression, ICT modulation and PET inhibition to generate highly selective “turn-on” or ratiometric fluorescence responses. The 1,2,3-triazole motif has become one of the most powerful scaffolds for Pb^{2+} detection due to its nitrogen-rich coordination environment, aromatic stabilization and synthetic modularity via CuAAC click chemistry. Literature examples including BSA-Trz and T1 highlight the ability of triazole-based probes to achieve ultralow nanomolar detection limits, reversible and reusable sensing, and multifunctionality, including bioimaging and molecular logic gate applications. Likewise, azo- and azine-based probes leverage their π -conjugated chromophores and electron-rich backbones to produce high-contrast optical responses, including visible colorimetric shifts and ratiometric fluorescence, often in aqueous media.

Beyond discrete molecular probes, porous hybrid materials such as MOFs and COFs provide extended sensing platforms with intrinsic structural order and high surface areas. Reports on Ti-, Zn-, and lanthanide-based MOFs demonstrate ratiometric sensing, highly reversible optical response, and femtomolar-to-nanomolar detection limits in aqueous conditions. Similarly, COFs and COPs (e.g., COF-CB, Pery-DHTP-BZ-COP) incorporate robust covalent linkages with tunable electron donor-acceptor frameworks, enabling selective quenching or fluorescence switching, high thermal stability, and recyclability, positioning them as promising next-generation Pb^{2+} optical sensors. Moving forward, the central challenges remain: (i) improving selectivity in complex biological and environmental samples containing multiple competing cations, (ii) enhancing probe water solubility and reducing

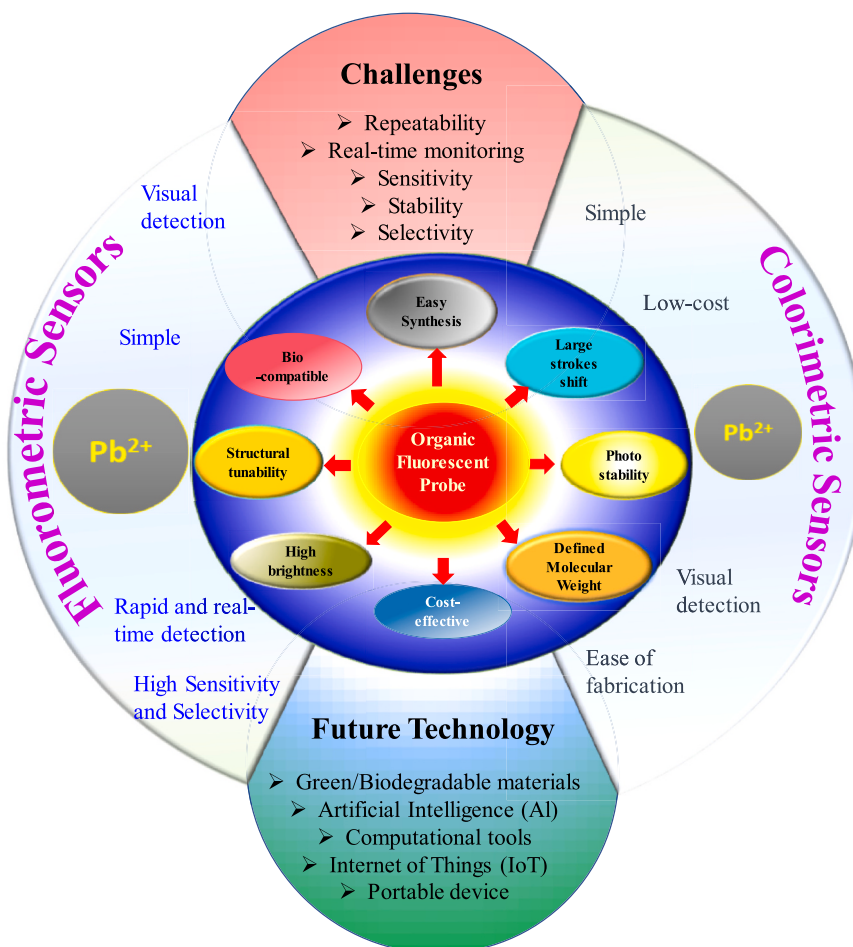


Fig. 21. Schematic illustration summarizing the future perspectives and design strategies for organic fluorescent Pb^{2+} sensors.

cytotoxicity for bioimaging applications, and (iii) integrating molecular chemosensors into real-world devices (Fig. 21). The translation of these sensing platforms into portable, cost-efficient, and smartphone-enabled analytical tools will be critical for real-time, on-site Pb^{2+} monitoring.

Looking ahead, computational chemistry and artificial intelligence are poised to play transformative roles in the rational design of next-generation Pb^{2+} probes. Molecular docking, DFT, and TD-DFT simulations can provide valuable insights into metal-ligand interactions and guide the prediction of optical responses before synthesis, while AI and machine learning algorithms can screen vast molecular libraries, optimize sensing performance, and identify new design principles. The integration of these computational approaches with experimental synthesis will greatly accelerate the development of highly selective, efficient, and sustainable Pb^{2+} sensors. Future research should also focus on combining the high sensitivity of fluorescence-based systems with the simplicity and accessibility of colorimetric detection. The incorporation of nanostructured materials, green chemistry strategies, and smart technologies such as AI- and IoT-enabled sensing networks will enable real-time, autonomous, and environmentally friendly Pb^{2+} detection. Collectively, these interdisciplinary advances promise to deliver scalable, reliable, and user-friendly sensing platforms, safeguarding environmental quality, food safety, and public health.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Data availability

Data will be made available on request.

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