Abstract

Research on developing new electron donor–acceptor (EDA) based molecular systems, which benefit from extended π-conjugation, is a rapidly growing research area. That has resulted in several technological applications, including fluorescent dyes, laser dyes, brightening agents, metal sensors, pH sensors, bio-imaging, organic photovoltaics (OPVs), organic light-emitting diodes (OLEDs), and many more. The photophysical properties of donor (**D**)-acceptor (**A**) based molecular systems depend on the substitution pattern and the **D-A** unit's nature, making them prime derivatives for application in organic photonics. The most frequent method for tuning the photophysical properties of organic compounds is to connect an electron-rich "**D**" and an electron-deficient "**A**" group directly or indirectly. The π-linkage between the "**D**" and "**A**" units results in a **D**-π-**A** type of conjugated molecular system, where the photophysical/electronic properties of **D**-π-**A** systems can be tuned by either (i) changing the "**D**" or "**A**" unit strength or (ii) varying the π-linker between the "**D**" and "**A**" units. A wide range of **D-A** conjugated systems with varying "**D**" and "**A**" units have been developed for various applications in chemistry, physics, materials science, and biology. Because of their superior photophysical characteristics, these are used to develop and create various sensory materials for monitoring biological events and detecting various target analytes. Chemosensors based on photoluminescence are essential among the many approaches and methodologies because they have multiple benefits, such as on-site detection, real-time monitoring with rapid response, innately high sensitivity, and simplicity of handling compared to other techniques. Considering the real benefit of the chromo-fluorogenic EDA system, present thesis explores its practical benefit for detection of various target analytes.

A brief summary of each chapter of the present thesis are given below one by one.

Chapter 1: This chapter begins with a brief discussion of the EDA system-based chemosensors and then moves to the general principle and working mechanism for designing chemosensors based on different photophysical processes with examples. This chapter deals with the objectives and applications of the present work in the present context of scientific development.

Chapter 2: This chapter explores the reversible acidochromic behavior of a benzoxazole-based scaffold (**BPP**), which is highly sensitive to the acid-base in the liquid and gas phases. With the addition of acid, the solution of **BPP** changes its color from yellow to pink fuchsia due to the transformation of its imine into quinonoid form. The color change is completely reversible in the presence of the base, confirming the reversible acidochromic behavior of the present **BPP** system. Further, a paper strips-based test kit has been demonstrated for the practical utility of the present acidochromic **BPP** to identify a trace amount of acid-base in solution and gas-phase, respectively. The mechanistic aspects of detecting acid-base and colorimetric change in the presence of acid-base

have been explored by density functional theoretical investigations and ^{1}H NMR experiments. Moreover, we have constructed a reconfigurable dual-output combinatorial **INH/IMP** logic gate.

Chapter 3: This chapter highlights the investigation of anion interactions and recognition abilities of naphthalene derivative, [(E)-1-(((4-nitrophenyl) imino) methyl) naphthalen-2-ol], (**NIMO**) by UV–visible spectroscopically and colorimetrically. **NIMO** shows selective recognition of F^{-} ions colorimetrically, and the naked eye observes a visual color change from yellow to pink. The F^{-} ions recognition is fully reversible in the presence of HSO_4^{-} ions. The limit of F^{-} ions detection by **NIMO** could be possible down to 0.033 ppm-level. A paper strips-based test kit has been demonstrated to detect F^{-} ions selectively by the naked eye, and a smartphone-based method for accurate sample analysis in the non-aqueous medium has also been demonstrated. The pK_a value calculation and DFT analysis support spectroscopic behavior to find a correlation with receptor analyte interaction. The optical response of **NIMO** towards the accumulation of F^{-} ions and, subsequently, HSO_4^{-} ions as chemical inputs provide an opportunity to construct **INH** and **IMP** molecular logic gates.

Chapter 4: In this chapter, a fluorosensor derived from 4-aminophthalimide, ((E)-5-((2-hydroxy benzylidene) amino) isoindoline-1, 3-dione, **HID** working with excited state intramolecular proton transfer (ESIPT) mechanism is synthesized and employed for the selective recognition of aluminum (Al^{3+}) ions and picric acid (PA) based on '*off-on-off*' fluorescence mechanism. The sensor **HID** shows a turn-on fluorescence response towards Al^{3+} ions in H_2O/DMSO (9:1, V/V) with a rapid response time (2 minutes) and exceptional sensitivity (LOD = 0.77 μM). The binding constant (K) of **HID** with Al^{3+} ions is estimated to be 1.32×10^{8} M^{-2}. The 1:2 stoichiometries of the complex between **HID** and Al^{3+} ions are confirmed through Job's plot and ^{1}H NMR spectral analysis. Al^{3+} chelated **HID** complex is further employed to detect explosive nitroaromatic compounds, especially PA. Furthermore, using these two chemically encoded inputs, and corresponding optical output, we constructed the INH molecular logic gate with Al^{3+} and PA. The **HID** chemosensor and Al^{3+} chelated **HID** complex are also applied to map Al^{3+} ions and PA in the living cell. The **HID** chemosensor and Al^{3+} chelated **HID** complex's performance toward detecting Al^{3+} ions, and PA demonstrates that it might be used as a signaling tool for analyzing biological and environmental samples.

Chapter 5: This chapter attempts to introduced a photoluminescence ionic liquid and its application for detecting nitro explosives. Due to the rising menace of illicit actions and pollution aroused by explosive nitroaromatic compounds (NACs), the growth of an adept sensor for detecting these NACs is essential. Herein, in this communication, a photoluminescent IL-assimilated group of uniform materials based on organic salt (GUMBOS) and Nano-GUMBOS has been fabricated by integrating pyrene butyrate with a quaternary phosphonium IL (**PbIL**) via a simple ion exchange process. Neat **PbIL** shows a bright cyan color photoluminescence under a 365 nm UV lamp irradiation and is employed as photoluminescence security ink and picric acid (PA) detection among the tested NACs. By simple reprecipitation method, we have developed water-suspended crystalline pyrene assimilated nanoparticles, **nPbIL,** characterized by various analytical techniques. The **PbIL**-derived water-suspended nanomaterials, **nPbIL,** display a robust cyan color excimer-like emission, which turns blue (monomeric) due to adding PA over the other related NACs. This ratiometric cyan-to-blue photoluminescence change is due to the displacement of the anionic pyrene moiety of the **nPbIL** by the picrate anion. The fabricated organo nanosensor is enormously discerning and responsive towards PA with a LOD of 0.77 nM and is superior to many available in the literature. Additionally, a fluorogenic paper strip-based test kit experiment has been demonstrated to detect and quantify PA selectively in aqueous solvents amongst the other tested NACs. The present contribution evokes a novel approach to developing different IL-based chemosensors for detecting and quantifying various target analytes.

Chapter 6: This chapter attempts to demonstrate the role of different mimics of G-series nerve agents and their detection method. There is a pressing need for rapid and accurate recognition of hazardous G-series nerve agents in the solution and vapor phases to protect individuals from undesirable wars and terrorist attacks. However, achieving this goal in practice presents significant challenges. This contribution introduces a specific and selective acridine-based fluorogenic sensor, **AMA**, which exhibits turn-on behavior from cyan to blue photoluminescence under the exposure of a 365 nm UV lamp in response to diethylchlorophosphate (DCP), a mimic of sarin gas, in both liquid and vapor phases, respectively. The mechanism underlying the identification of DCP using **AMA** has been elucidated through ^{1}H-NMR titration investigation and HRMS analaysis. The fluorgenic, DCP-specific **AMA** shows an outstanding selectivity, excellent sensitivity, and a broad linear span of 15-38 μM, with an identification limit of 7.9 nM, which is found to be superb than many chemosensors available in the literature without any interference. To facilitate its potential practical applications, we have introduced an **AMA**-coated test kit utilizing Whatman-41 filter paper, which can be used as a handy and visual photonic device for on-spot identification of DCP as a mimic for sarin gas under the colonial crowding condition of other analogous analytes. Furthermore, we have demonstrated a fluorogenic dip-stick method to detect and quantify the DCP vapor under the exposure of a 365 nm UV lamp.

Chapter VII: Finally, a brief summary of the present thesis and the future perspective from the present research work has been delineated in this chapter.