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Sustainable Science and Technology **Extended Abstract**

Track (SM)

N-Doped Carbon Dots for Visual Recognition of 4-Nitroaniline and Use in Fluorescent Inks

Nilanjana Nandi, [a] Priyanka Sarkar, [a] Kalyanasis Sahu[*a]

*Department of Chemistry, Indian Institute of Technology Guwahati, Guwahati 781039, Assam, India

*Corresponding author E-mail: ksahu@iitg.ac.in (K.S.).

ABSTRACT: Carbon dot (CD)-based fluorometric detection of the industrial pollutant, 4-nitroaniline (4-NA), is a very challenging research arena. We designed two N-doped CDs (NCDs) with distinct photophysical characteristics by varying the heteroatom percentage. The CD emission color shifts from blue (NCD-1) to green (NCD-2) in water as the heteroatom percentage increases from 8.3% to 15.8%. The NCDs also slightly differ in size with diameters of 2.5 and 3.6 nm, respectively. In comparison to NCD-2, only NCD-1 exhibits bright green luminescence (521 nm) in the solid state. The as-prepared NCDs showed excellent solvent-dependent emission behavior; NCD-2 shows a higher spectral shift (76 nm) than NCD-1 (41 nm) as the solvent medium changes from tetrahydrofuran (THF) to water. NCD-2 displays blue emission in DMSO and green emission in water. Both NCDs perform excellently for discriminative recognition of 4-NA by fluorescence quenching. Detailed investigation revealed that quenching mechanisms depend on the distinct fluorescence properties of NCDs and the solvent medium. In water, NCD-1 fluorescence mainly quenches through inner filter effect (IFE) and photoinduced electron transfer (PET), while a combination of Förster resonance energy transfer (FRET) and PET account for the fluorescence quenching of NCD-2. In the DMSO medium, the primary fluorescence quenching pathways of NCD-2 were FRET and IFE, along with a small contribution of PET. Furthermore, an inexpensive portable paper strip was constructed to demonstrate a fast and easy on-site sensing of 4-NA. Additionally, newly developed NCDs were ideal for application in the arena of invisible ink.

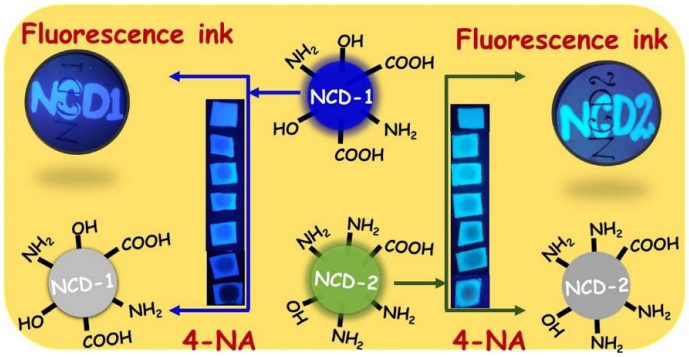


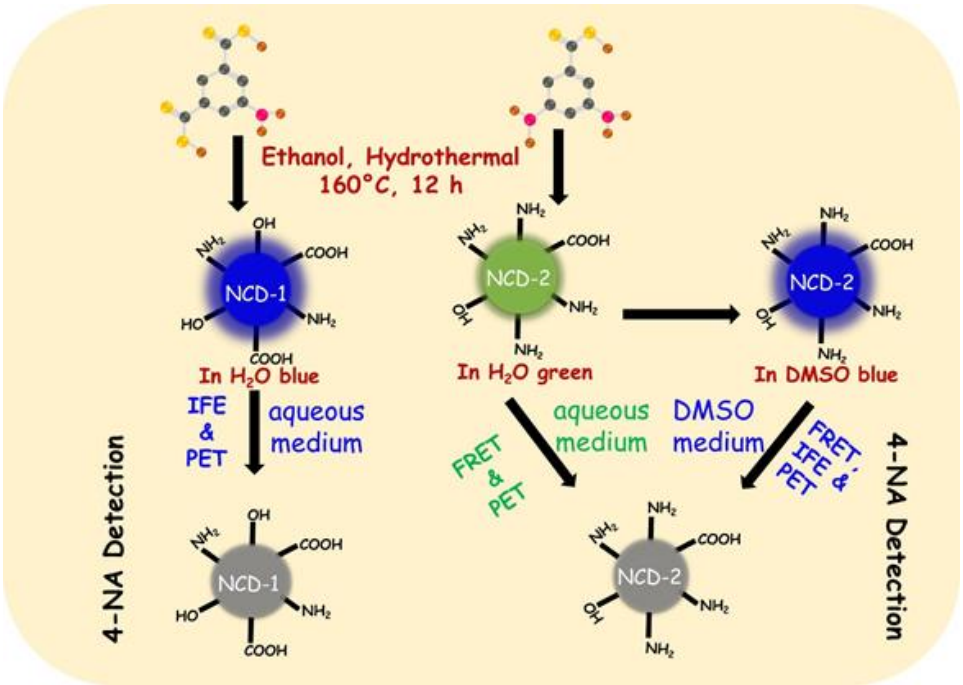
Table of content. Schematic representation of detection of 4-NA by NCD-1 and NCD-2.

Results

- In this report, two nanodots NCD-1 and NCD-2, with varying N-content, have been synthesized with blue and green emissions in an aqueous medium through a cost-effective, one-pot hydrothermal method.

- The FL properties of the NCDs have different prospects; NCD-1 has outstanding solid-state emission properties while NCD-2 exhibits different color emissions in water (green) and DMSO (blue).
- Interestingly, the fluorescence quenching mechanisms differ in each case; for NCD-1 in water, PET and IFE dominate, whereas FRET and PET are crucial for NCD-2 in water, and all three FRET, IFE, and PET operate together for NCD-2 in DMSO medium.
- Additionally, two NCD systems were applied for real sample analysis as well as paper strip-based detection of 4-NA, revealing promising results. Furthermore, both the NCDs can be effectively applied as an efficient fluorescent ink application.
- For more details, we provide a table for better understanding the sensing mechanisms

Synthesized nanodots	Solvent	FL property	Primary detection mechanism	Secondary detection mechanism	Additional detection mechanism
NCD-1 (Blue emission)	Water	Excitation: 330 nm Emission: 430 nm	IFE (~ 55%)	PET	
NCD-2 (Green emission)	Water	Excitation: 410 nm Emission: 490 nm	FRET (~ 69%)	PET	IFE (~2%)
NCD-2 (Blue emission)	DMSO	Excitation: 350 nm Emission: 425 nm	FRET (~ 58%)	IFE (~ 37%)	PET



Scheme 1. Synthesis route and whole sensing pathways of 4-NA by NCD-1 and NCD-2.