Electronic Supplementary Information

Picric Acid sensing by Carbon Nanodots: Theoretical Validation of Selectivity

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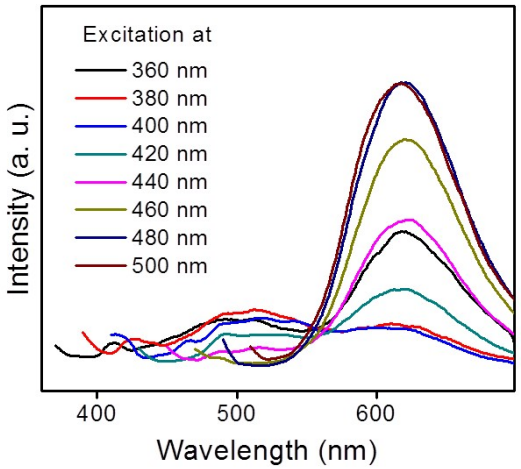


Figure S1: Excitation dependent emission of PD-CNDs

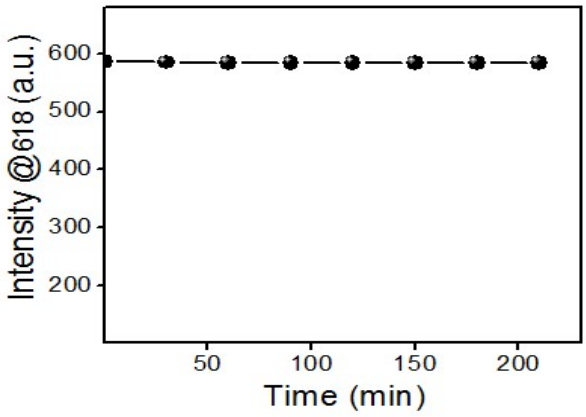
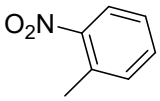
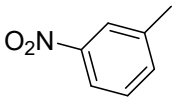
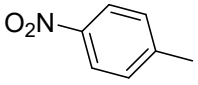
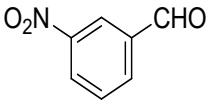
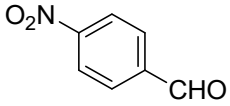
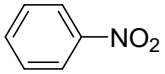
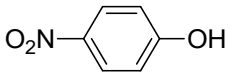
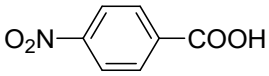
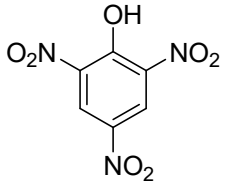
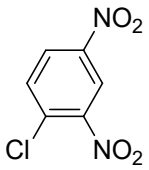


Figure S2: Photostaility of PD-CNDs under continuous UV illumination

Table S1: Details of selected analytes for the studies

No	Compound	Abbr.	Molecular weight	Structure
1	o-Nitrotoluene	o-NT	137.14	
2	m-Nitrotoluene	m-NT	137.14	
3	p-Nitrotoluene	p-NT	137.14	
4	m-Nitrobenzaldehyde	m-NBZA	151.12	
5	p-Nitrobenzaldehyde	p-NBZA	151.12	
6	Nitrobenzene	NB	123.11	
7	p-Nitrophenol	p-NP	139.11	
8	p-Nitrobenzoic acid	p-NBA	167.12	
9	Picric acid	PA	229.11	
10	1-chloro-2,4-dinitrobenzene	CDNB	202.55	

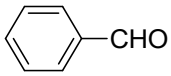
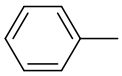
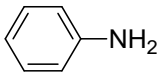
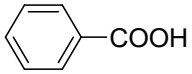
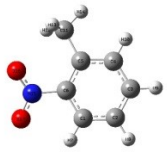
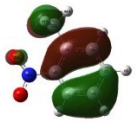
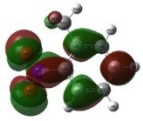
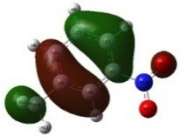
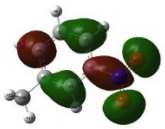
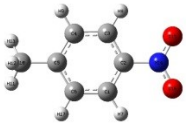
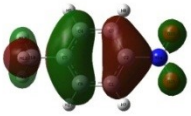
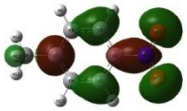
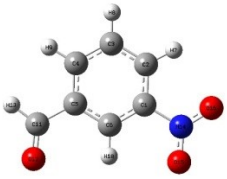
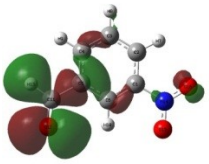
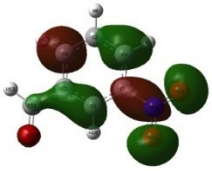
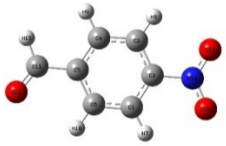
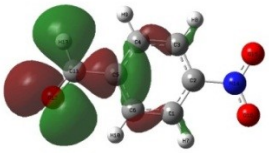
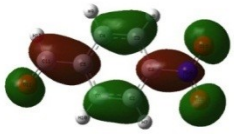
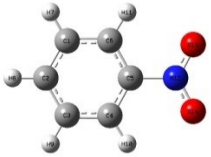
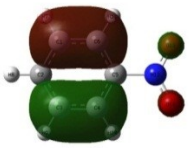
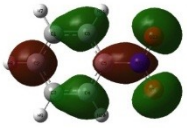
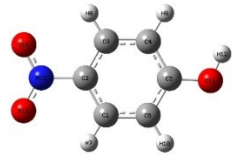
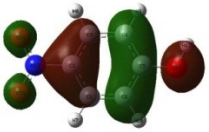
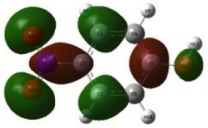
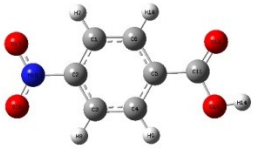
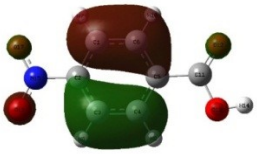
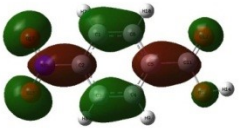
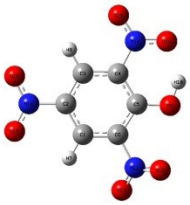
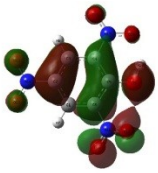
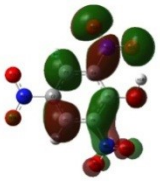
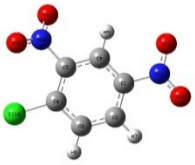
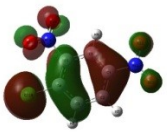
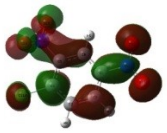
11	Benzaldehyde	BZA	106.12	
12	Toluene	T	92.14	
13	Aniline	A	93.14	
14	Benzoic acid	BA	122.12	

Table S2: Optimized geometries and HOMO / LUMO of selected nitroaromatic compunds

Compound	HOMO	LUMO
 *o*-NT		
 *m*-NT		
 *p*-NT		
 *m*-NBZA		
 *p*-NBZA		
 NB		

 *p*-NP		
 *p*-NBA		
 PA		
 CDBA		

Cyclic voltammetry measurements for determining the energy levels

The HOMO and LUMO energy levels of PD-CNDs could be estimated according to the empirical formula:

$$E_{HOMO} = -e(E_{ox}+4.4) \quad (1)$$

$$E_{LUMO} = -e(E_{red}+4.4) \quad (2)$$

Where E_{ox} and E_{red} are the onset of oxidation and reduction potential for PD-CNDs respectively. The E_{red} was determined to be -0.21 V. The corresponding E_{LUMO} was calculated to be -4.19 eV. To determine the HOMO levels, we combined the E_{red} with the optical energy band gap (E_g, resulting from the absorption edge in the absorption spectrum):

$$E_{HOMO} = E_{LUMO} - E_g \quad (3)$$

E_g was estimated to be 2.41 eV. So, the E_{HOMO} was calculated to be -6.60 eV.

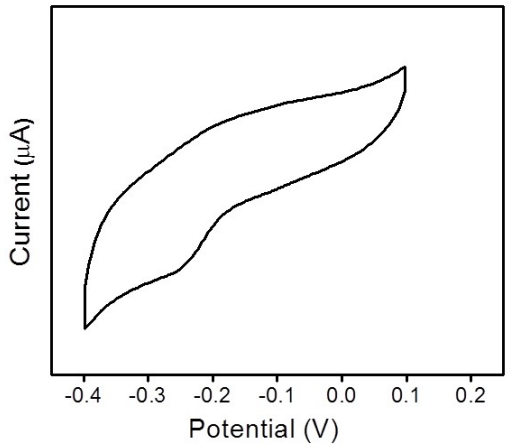


Figure S3: Cyclic voltammogram of PD-CNDs

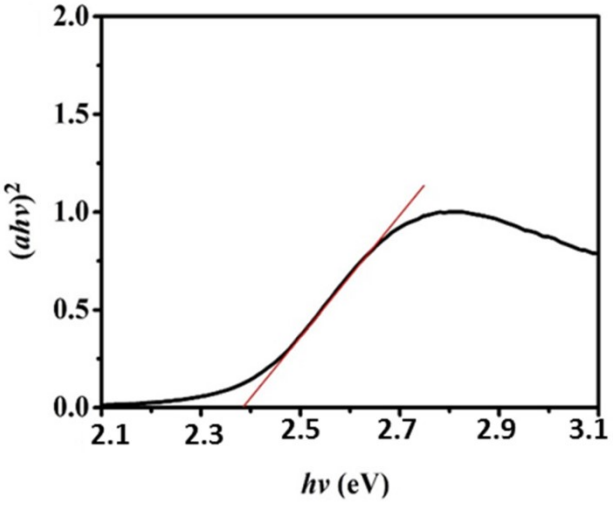


Figure S4: Tauc plot derived from UV Visible absorbance spectrum of PD-CNDs