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## **Supplementary Information**

# Enhancement in Room Temperature Ammonia Sensing Properties of Naphthalene Diimides through Core Expansion

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#### -1300 1200 -1100 -1000 900 800 700 600 500 400 300 -200 100 8 4.59 --100 6.5 6.0 4.5 2.0 0.5 10.0 9.5 8.5 8.0 7.5 7.0 5.5 5.0 f1 (ppm) 3.5 3.0 2.5 1.0 9.0 4.0 1.5

### NMR of NDI-CN<sub>4</sub>:

### NMR of NDI-H<sub>4</sub>:



Recyclability studies of NDI-CN<sub>4</sub> sensor towards various concentrations of ammonia



Fig. S1: Response of NDI-CN4 towards various concentrations of ammonia

Cyclic voltammetry study of NDI-H<sub>4</sub> and NDI-CN<sub>4</sub>



**Fig. S2:** Cyclic voltammograms of (a)NDI-H<sub>4</sub> and (b) NDI-CN<sub>4</sub>, run in dichloromethane (DCM) at a sweep rate of 50 mV per second.

**Table S1.** Frontier molecular orbital energies as estimated from cyclic voltammetry and optical absorption

Materials	E <sub>red onset</sub>	LUMO (eV)	HOMO (eV)	$\lambda_{abs onset}$	E <sub>g</sub> (eV)
NDI-H <sub>4</sub>	-1.18	-3.22	-6.58	368 nm	3.36
NDI-CN <sub>4</sub>	-0.21	-4.19	-6.33	578 nm	2.14

The details of calculations regarding  $E_{red onset}$ , HOMO/LUMO levels,  $\lambda_{abs onset}$  and  $E_g$  (eV) are given in the previous reports.<sup>1,2</sup>

- Y. Hu, X. Gao, C.-a. Di, X. Yang, F. Zhang, Y. Liu, H. Li and D. Zhu, *Chem. Mater.*, 2011, 23, 1204-1215.
- 2. L. Leonat, G. Sbarcea and I. V. Branzoi, UPB Sci Bull Ser B, 2013, 75, 111-118.