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The rapid-response room temperature planar type gas sensor based on the DPA-Ph-DBPzDCN for sensitive detection of NH_3

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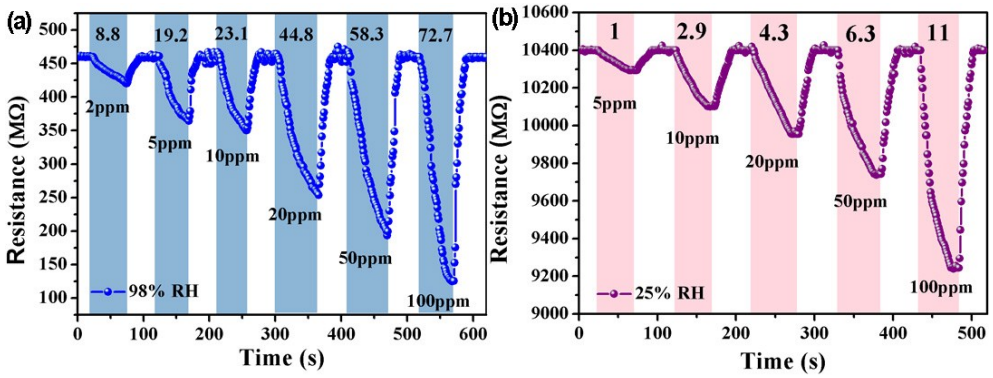

Fig.S1. (a) The response transients of the device based on DPA-Ph-DBPzDCN to 2-100 ppm NH_3 at room temperature and the 98% RH; (b) The response transients of the device based on DPA-Ph-DBPzDCN to 5-100 ppm NH_3 at room temperature and the 25% RH.

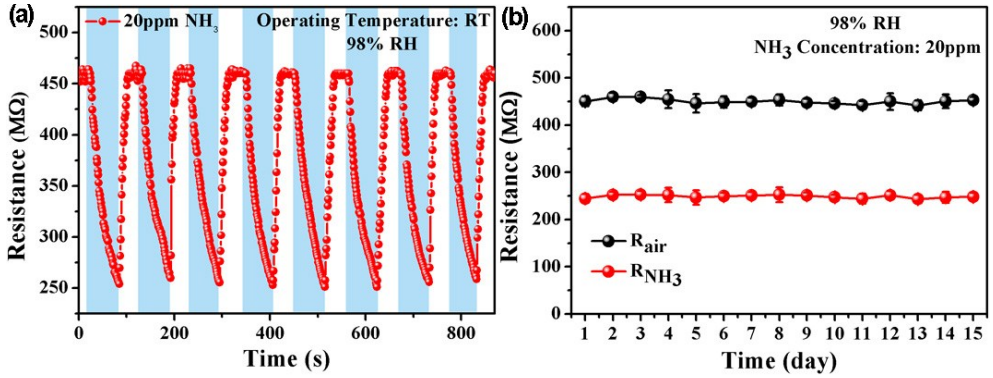

Fig.S2. (a) Repeatability of the response of the DPA-Ph-DBPzDCN sensors to 20 ppm NH_3 at room temperature and the 98% RH; (b) Stability of the DPA-Ph-DBPzDCN sensor stored unencapsulated at room temperature and the 98% RH for 15 days.

All DFT calculations were performed based on a level of GGA-UBLYP/DNP implemented in DMol3 code. Hydrogen bonding and van der Waals (vdW) interactions were semi-empirically estimated by a Tkatchenko-Scheffler (TS) scheme.[1]

Table.S1. The DFT calculated absorption energies of NH_3 and H_2O molecules on the DPA-Ph-DBPzDCN.

Configuration	Adsorption Energy (eV)		Adsorption Distance (Å)	
Gas species	NH_3	H_2O	NH_3	H_2O
A: Trihpenylamine-N	0.56	0.30	2.17	2.02
B: Dazine-N	0.41	0.22	2.19	2.11
C: Cyan-N	0.39	0.26	2.28	2.07

References

1. Tkatchenko and M. Scheffler, *Physical Review Letters*, 2009, **102**, 073005.