

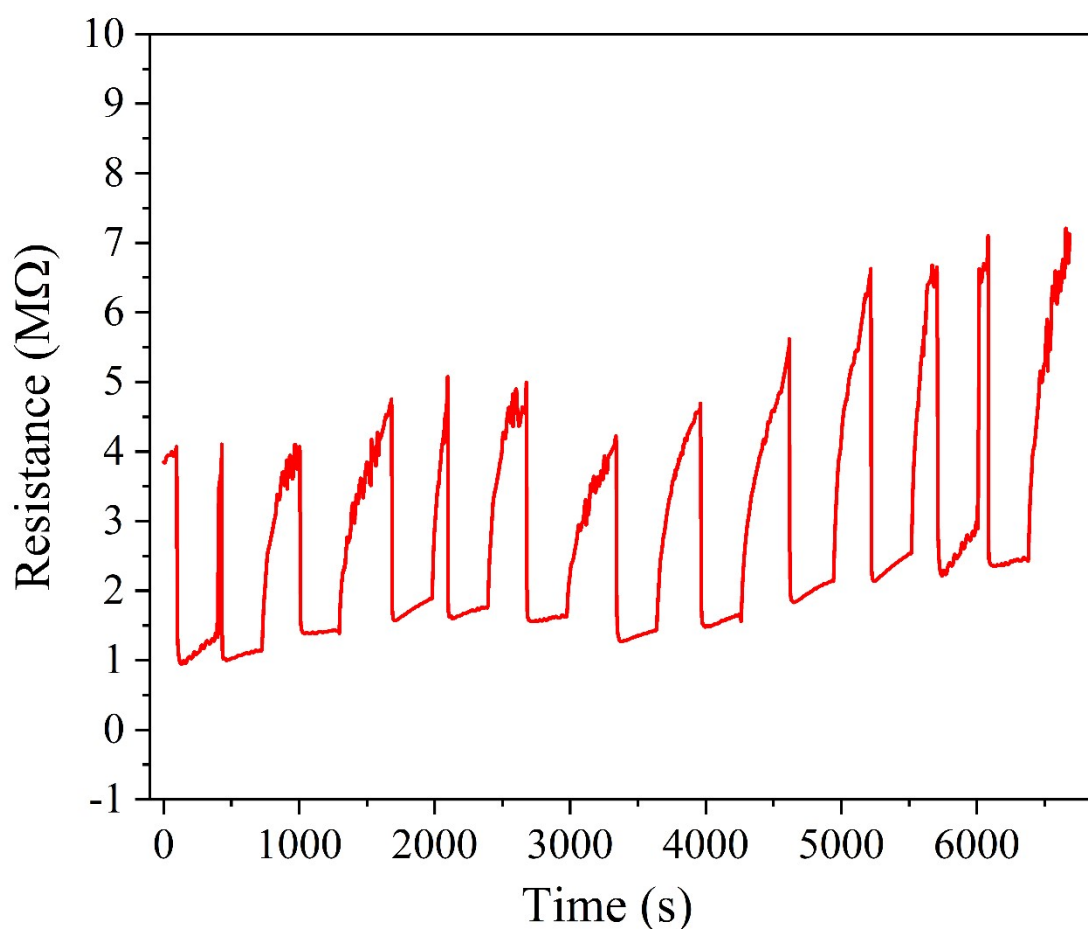
Electronic Supplementary Information for:

## N-doped graphdiyne derivative for highly selective and ultrasensitive NH<sub>3</sub> sensing at room temperature

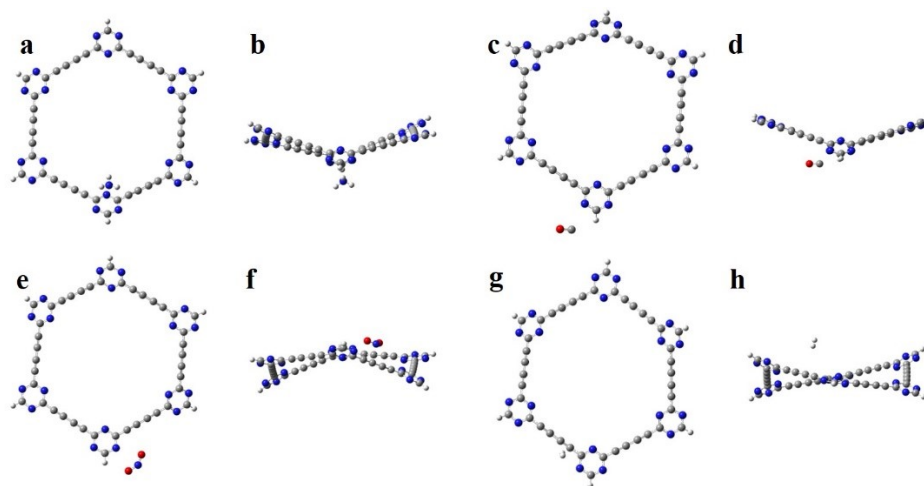
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**Fig. S1** Long-term response stability of N-GDYD for 100 ppm NH<sub>3</sub>.



**Fig. S2** Top view of optimized N-GDYD structure for model molecules interact with (a) NH<sub>3</sub>, (c) CO, (e) NO<sub>2</sub>, (g)H<sub>2</sub>; the side view of the optimized N-GDYD structure for the model molecule interacts with (b) NH<sub>3</sub>, (d) CO, (f) NO<sub>2</sub>, (h)H<sub>2</sub>. The grey, blue, white, and red ball represent for the carbon, nitrogen, hydrogen, and oxygen atom, respectively.