Supporting information for

An ammonia detecting mechanism of organic transistors revealed from recovery processes

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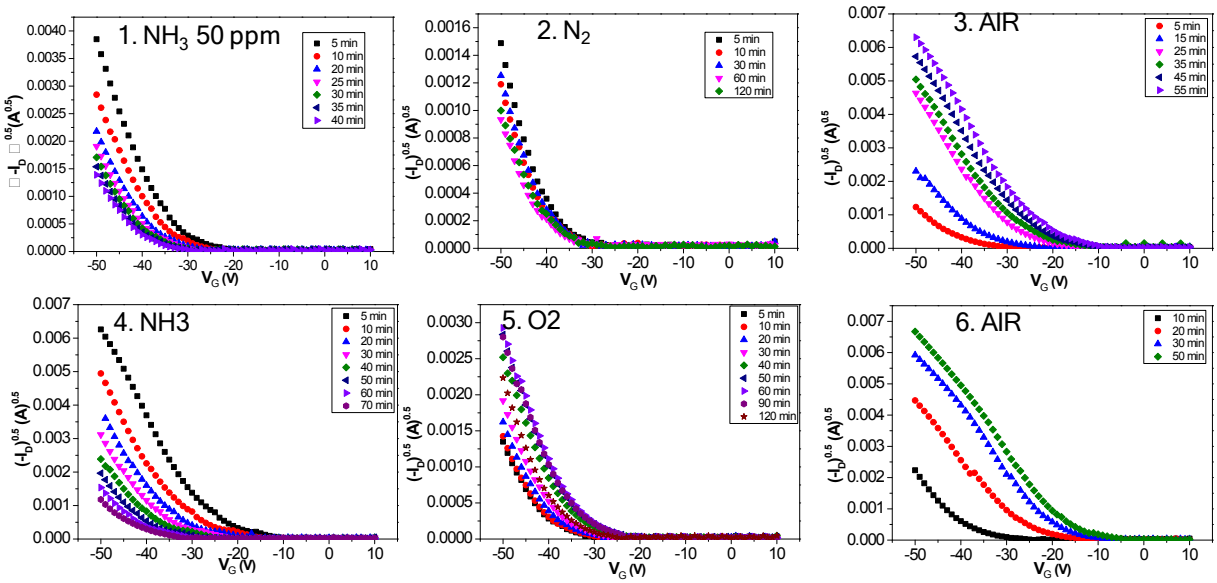
S1: Transfer curves of The DTBDT-C_9 thin film transistor in different atmospheres



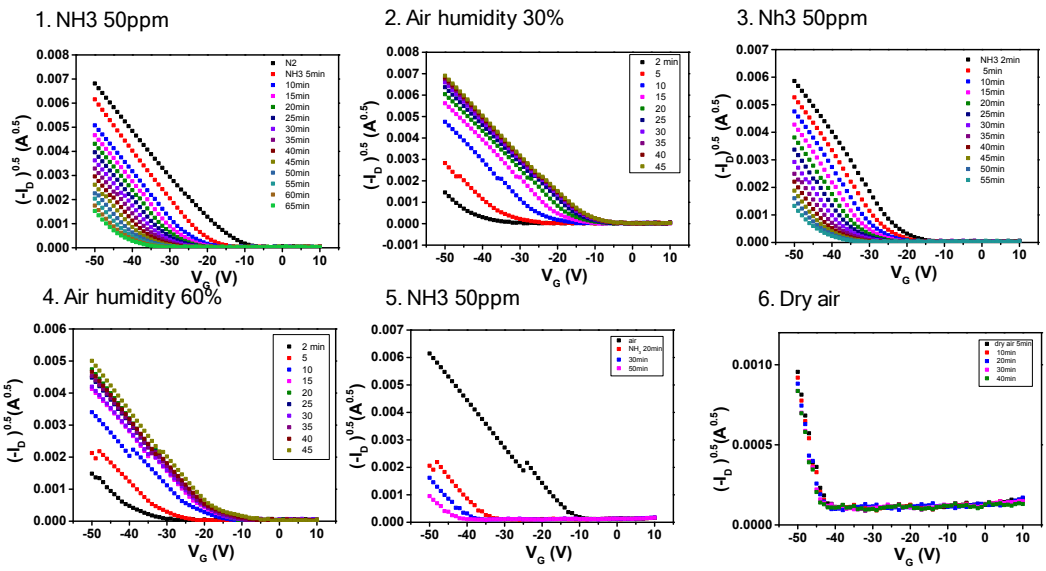


Figure S1. a) The transfer curves of DTBDT-C_9 transistors under exposure of the circle of NH_3-N_2-NH_3-Air-NH_3-O_2 -Air as a function of time; b) The transfer curves of DTBDT-C_9 transistors under exposure of the circle of NH_3-Air (RH 30%) -NH_3-Air (RH 60%)-NH_3-Air (RH 0%) as a function of time.

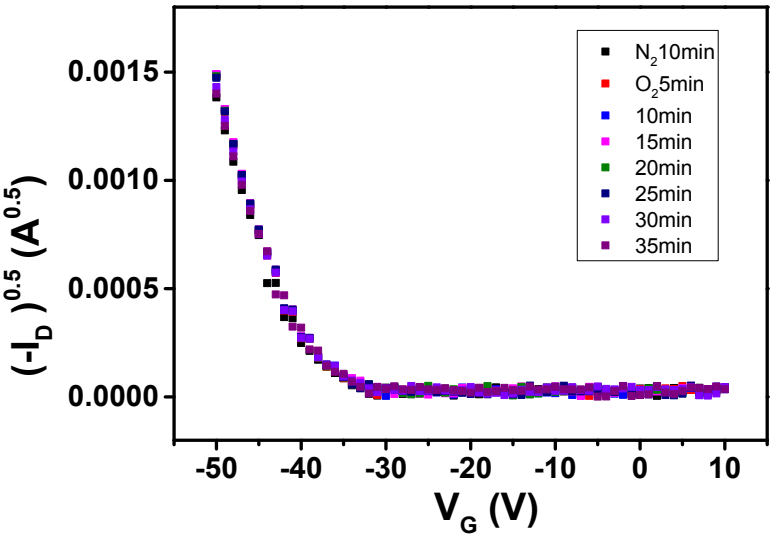


Figure S2. The transfer curves of a DTBDT-C_9 FET sensor upon exposure to O_2(RH0%) as a function of time.

S2: Evolution of the transistor performance response to NH_3 and recovery in dry CO_2 and wet CO_2

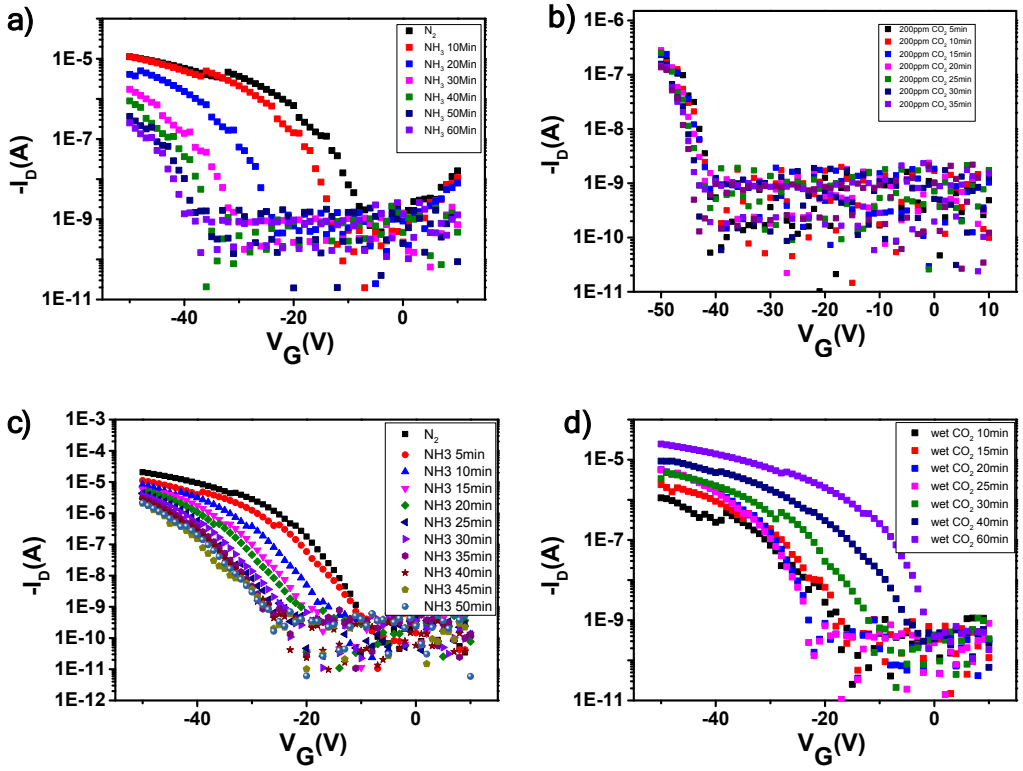


Figure S3. The transfer curves of transistor a) response to NH_3 atmosphere, b) recovery in dry CO_2, c) response to NH_3 atmosphere, d) recovery in wet CO_2.

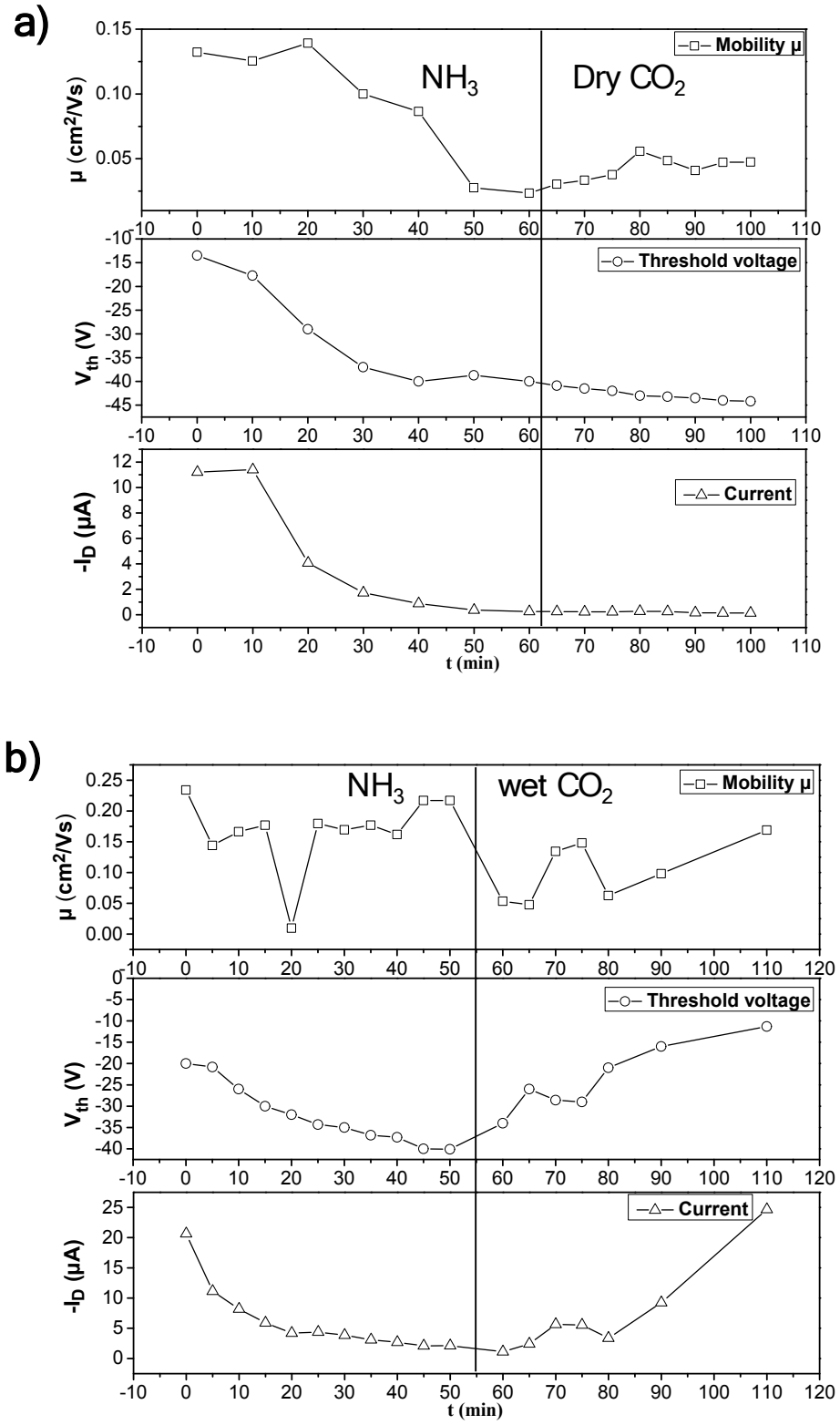


Figure S4. The transistor parameters evolution in the response and recovery process. a） response to NH_3 and then recovery in dry CO_2, b) response to NH_3 and then recovery in wet CO_2. The dark line in the figure marked the time that transferred the

atmosphere.

S3: Transfer curves of The DTBDT-C_9 thin film transistor on OTS modified substrates.

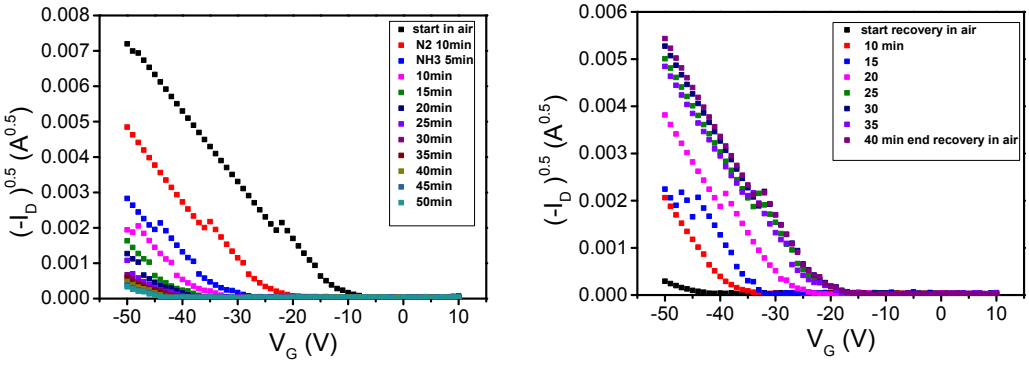


Figure S5. The transfer curves of a OTS modified DTBDT-C_9 FET sensor under exposure of the circle of NH_3(50ppm)- air(RH30%) as a function of time.

S4. DFT calculation

Calculation method and details: VASP code, GGA-PBE pseudopotential, vdW-D3 method, energy cutoff 400eV, change of total free energy 0.01 eV, 20 Å vacuum layer, 1× 1 × 1 k-mesh for geometry optimization, 3 × 3 × 1 k-mesh for electronic property calculations.

Table S1.

Configuration	Adsorption Energy/eV	
Gas species	NH_3	H_2O
A: center of thiophene	-0.16	-0.21
B: center of benzene	-0.15	-0.21
C: side to C-H bond	-0.18	-0.19

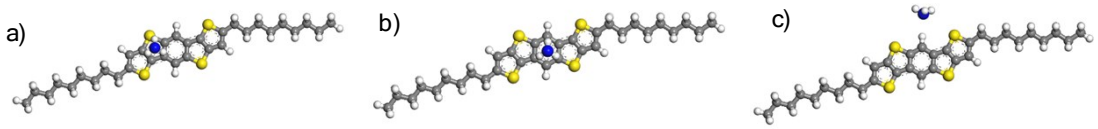


Figure S6. The three absorption configuration of the NH_3 molecule on the DTBDT-C_9 molecules.

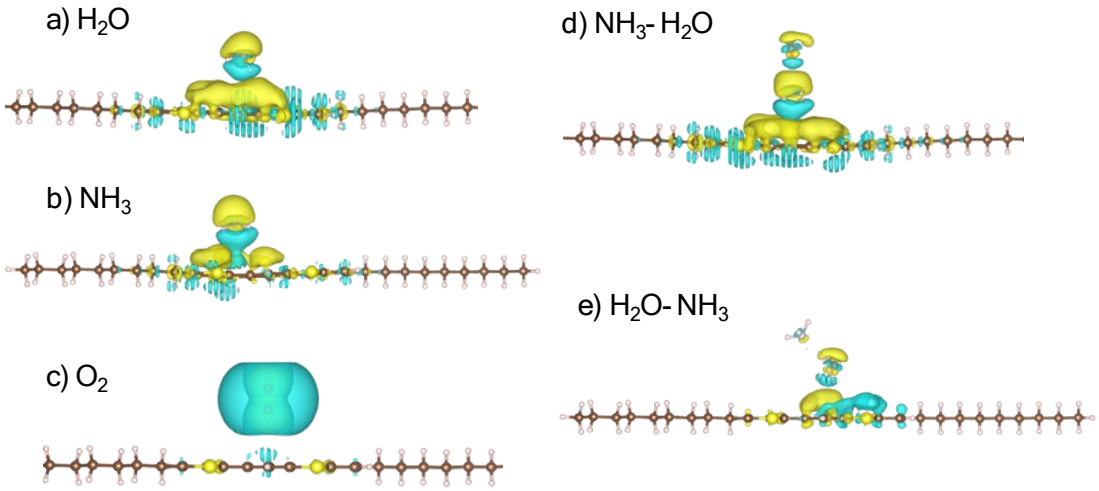


Figure S7. The charge density differences of the gas molecule absorbed on the DTBDT-C_9 molecules. a) H_2O, b) NH_3, c) O_2, d) NH_3 on DTBDT-C_9 pre-absorbed H_2O, e) H_2O on DTBDT-C_9 pre-absorbed NH_3