Supplementary Information

Backside fluorine-functionalized graphene layer for ammonia detection

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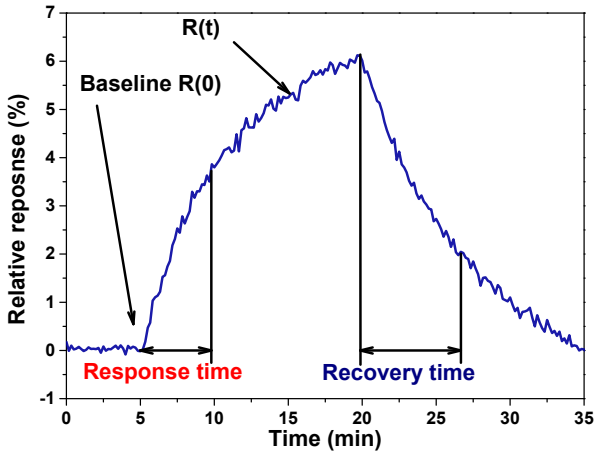

Figure S1. The main stages of the sensor interaction with an analyzing gas.

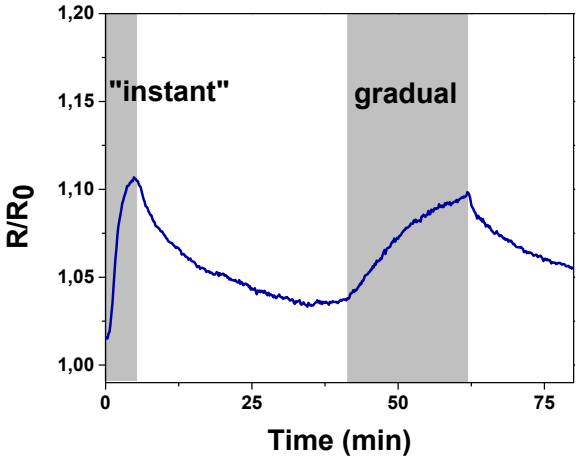

Figure S2. Response to 1 % of NH_3: first cycle – the sensor placed directly into the atmosphere of ammonia, second cycle – the necessary concentration achieved in a flow reactor.

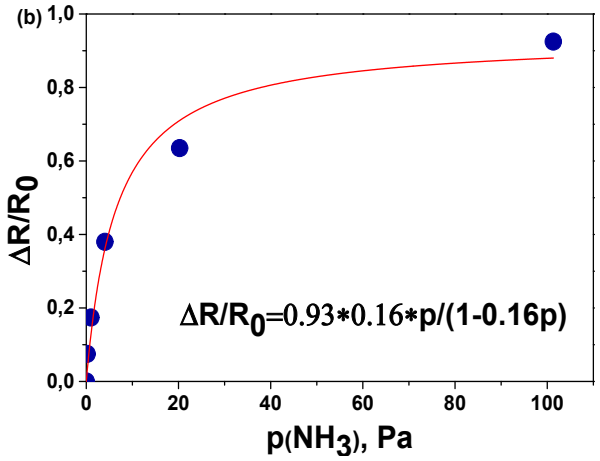

Figure S3. Dependence of sensor response of CVD-graphene on the NH_3 pressure. The curve was plotted using the experimental data presented in Fig. 2(a) in Ref. [F. Yavari, E. Castillio, H. Gullapalli, P.M. Ajayan and N. Koratkar, *Appl. Phys. Lett.,* 2012, **100**, 203120].

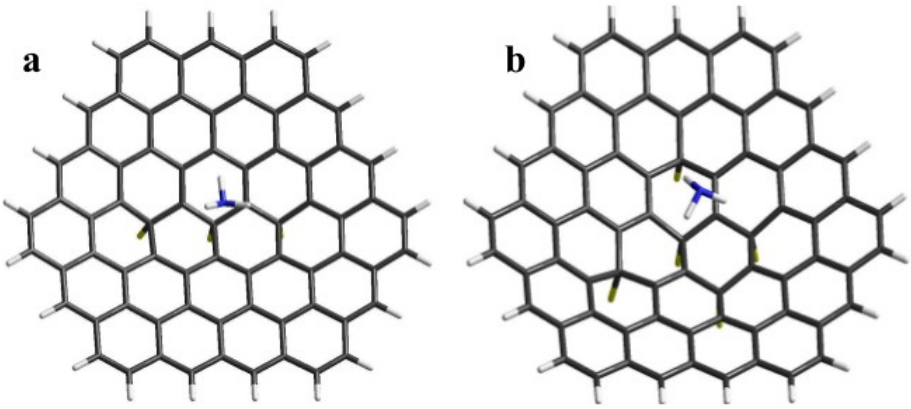

Figure S4. Geometry of models $C_{73}F_3H_{21}$ (a) and $C_{73}F_5H_{21}$ (b) showing less preferable mutual orientation of NH_3 molecule relative to fluorinated graphene surface. In the model, $C_{73}F_3H_{21}$ the molecule approaches by N and H atoms – $C_{73}\mathbf{F_3}H_{21}(NH_3)$ configuration in Table S1; in the model $C_{73}F_5H_{21}$, the molecule approaches by three hydrogen atoms – $C_{73}\mathbf{F_5}H_{21}(H_3N)$ configuration in Table S1.

model	$C_{73}\mathbf{F}H_{21}$	$C_{73}\mathbf{F_3}H_{21}(H_3N)$	$C_{73}\mathbf{F_3}H_{21}(NH_3)$	$C_{73}\mathbf{F_5}H_{21}(H_3N)$	$C_{73}\mathbf{F_5}H_{21}(NH_3)$
distance	2.86 (C-H_1) 2.88 (C-H_2) 2.90 (C-H_3)	2.66 (C-H_1) 2.70 (C-H_2) 2.87 (C-H_3)	2.96 (C-H) 2.99 (C-N)	2.97 (C-H_1) 3.00 (C-H_2) 3.04 (C-H_2)	2.93 (C_1-H_1) 2.94 (C_2-H_1) 3.06 (C_1-H_2)

Table S1 The distance between atoms in a molecule and the nearest surface atoms (Å) for "hydrogen" (H_3N) or "nitrogen" (NH_3) orientation of the molecule.

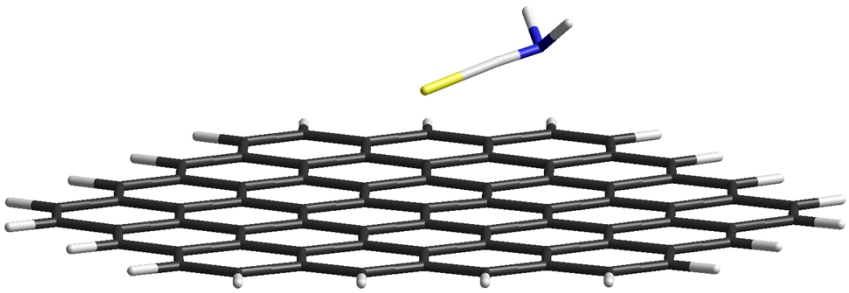

Figure S5. Charge-transfer complex of graphene and F–HNH_2 species obtained as the result of interaction of NH_3 molecule with fluorine atom in $C_{73}FH_{21}$ model. The shortest C–F distance is 2.4 Å. The length of the F–H bond is 1.7 Å that corresponds to hydrogen bonding.