Supporting Information

Two-dimensional C_3N based sub-10 nanometer Biosensor

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Table S1: Abbreviations used for naming different configurations of the C_3N Nanoribbon

Sr. No.	Symbols	Nomenclature description of symbols
1	Z_P	Zigzag monolayer of C_3N
2	Z_{PA}	Adenine molecule attached on the edge of Zigzag monolayer of C_3N
3	Z_{PC}	cytosine molecule attached on the edge of Zigzag monolayer of C_3N
4	Z_{PG}	Guanine molecule attached on the edge of Zigzag monolayer of C_3N
5	Z_{PT}	Thymine molecule attached on the edge of Zigzag monolayer of C_3N
6	Z_{PU}	Uracil molecule attached on the edge of Zigzag monolayer of C_3N
7	Z_{MB}	Boron doping at middle of Zigzag C_3N monolayer
8	Z_{MBA}	Adenine molecule attached on the edge of middle Boron doped Zigzag C_3N layer
9	Z_{MBC}	Cytosine molecule attached on the edge of middle Boron doped Zigzag C_3N layer
10	Z_{MBG}	Guanine molecule attached on the edge of middle Boron doped Zigzag C_3N layer
11	Z_{MBT}	Thymine molecule attached on the edge of middle Boron doped Zigzag C_3N layer
12	Z_{MBU}	Uracil molecule attached on the edge of middle Boron doped Zigzag C_3N layer
13	Z_{MSA}	Adenine molecule attached on the edge of middle Sulphur doped Zigzag C_3N layer
14	Z_{MSC}	Cytosine molecule attached on the edge of middle Sulphur doped Zigzag C_3N layer
15	Z_{MSG}	Guanine molecule attached on the edge of middle Sulphur doped Zigzag C_3N layer
16	Z_{MST}	Thymine molecule attached on the edge of middle Sulphur doped Zigzag C_3N layer
17	Z_{MSU}	Uracil molecule attached on the edge of middle Sulphur doped Zigzag C_3N layer
18	Z_{EBA}	Adenine molecule attached on the side of middle Boron doped Zigzag C_3N layer
19	Z_{EBC}	Cytosine molecule attached on the side of middle Boron doped Zigzag C_3N layer
20	Z_{EBG}	Adenine molecule attached on the side of middle Sulphur doped Zigzag C_3N layer
21	Z_{EBT}	Adenine molecule attached on the side of middle Sulphur doped Zigzag C_3N layer
22	Z_{EBU}	Adenine molecule attached on the side of middle Sulphur doped Zigzag C_3N layer
23	Z_{ESA}	Adenine molecule attached on the side of middle Sulphur doped Zigzag C_3N layer
24	Z_{ESC}	Adenine molecule attached on the side of middle Sulphur doped Zigzag C_3N layer
25	Z_{ESG}	Adenine molecule attached on the side of middle Sulphur doped Zigzag C_3N layer
26	Z_{EST}	Adenine molecule attached on the side of middle Sulphur doped Zigzag C_3N layer
27	Z_{ESU}	Adenine molecule attached on the side of middle Sulphur doped Zigzag C_3N layer
28	Z_{DV}	C_3N monolayer having double vacancy defect
29	Z_{DVA}	Adenine molecule attached on the edge of C_3N monolayer having double vacancy defect
30	Z_{DVC}	Cytosine molecule attached on the edge of C_3N monolayer having double vacancy defect
31	Z_{DVG}	Guanine molecule attached on the edge of C_3N monolayer having double vacancy defect
32	Z_{DVT}	Thymine molecule attached on the edge of C_3N monolayer having double vacancy defect
33	Z_{DVU}	Uracil molecule attached on the edge of C_3N monolayer having double vacancy defect
34	Z_{SV}	C_3N monolayer having single vacancy defect
36	Z_{SVA}	Adenine molecule attached on the edge of C_3N monolayer having single vacancy defect
37	Z_{SVC}	Cytosine molecule attached on the edge of C_3N monolayer having single vacancy defect
38	Z_{SVG}	Guanine molecule attached on the edge of C_3N monolayer having single vacancy defect
39	Z_{SVT}	Thymine molecule attached on the edge of C_3N monolayer having single vacancy defect
40	Z_{SVU}	Uracil molecule attached on the edge of C_3N monolayer having single vacancy defect
41	Z_{SW}	C_3N monolayer having stone wales defect
42	Z_{SWA}	Adenine molecule attached on the edge of C_3N monolayer having stone wales defect
43	Z_{SWC}	Cytosine molecule attached on the edge of C_3N monolayer having stone wales defect
44	Z_{SWG}	Guanine molecule attached on the edge of C_3N monolayer having stone wales defect
45	Z_{SWT}	Thymine molecule attached on the edge of C_3N monolayer having stone wales defect
46	Z_{SWU}	Uracil molecule attached on the edge of C_3N monolayer having stone wales defect
47	Z_{A1}	adenine molecule attached on the one side of Zigzag C_3N monolayer
48	Z_{A2}	First adenine attached on one side and Second adenine molecule attached on other side of Zigzag C_3N monolayer
49	Z_{A3}	One adenine attached on one side and two adenine molecule attached on other side of Zigzag C_3N monolayer
50	Z_{A4}	Two-Two adenine attached on both side of Zigzag C_3N monolayer
51	Z_P ($V_g = 0$ V)	Zigzag monolayer of C_3N at zero gate voltage
52	Z_{PA} ($V_g = 0$ V)	Adenine molecule attached on the edge of Zigzag monolayer of C_3N at zero gate voltage

53	Z_P (V_g = 10 V)	Zigzag monolayer of C_3N at gate voltage of 10 V
54	Z_{PA} (V_g = 10 V)	Adenine molecule attached on the edge of Zigzag monolayer of C_3N at zero gate voltage of 10 V
55	Z_P (V_g = 20 V)	Zigzag monolayer of C_3N at zero gate voltage of 20 V
56	Z_{PA} (V_g = 20 V)	Adenine molecule attached on the edge of Zigzag monolayer of C_3N at zero gate voltage of 20 V

A. System of zigzag polyaniline nanoribbon

We calculated the transport properties of C_3N nanoribbon and analysed the effect of DNA molecules attached to the edge of C_3N.

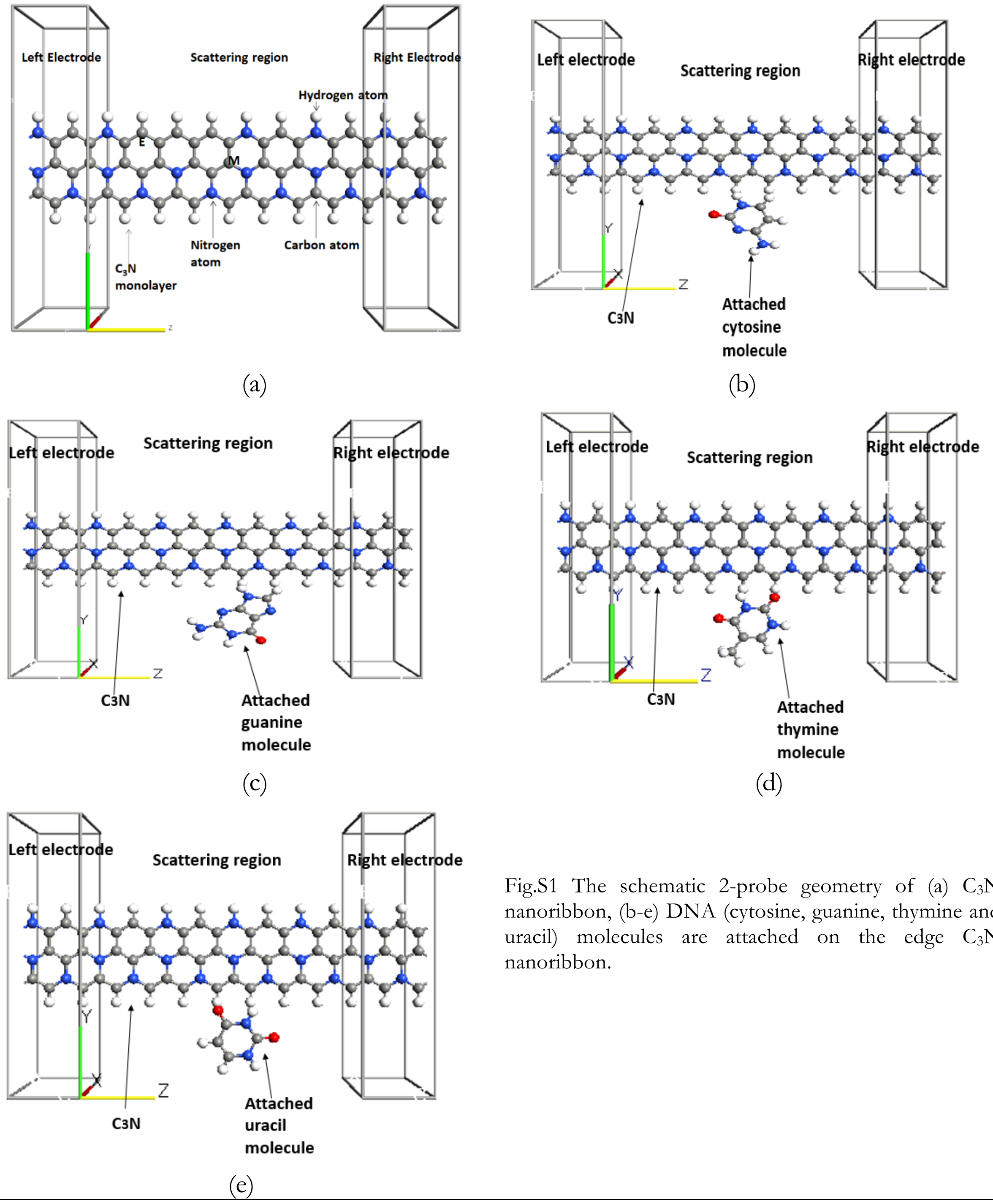

Fig.S1 The schematic 2-probe geometry of (a) C_3N nanoribbon, (b-e) DNA (cytosine, guanine, thymine and uracil) molecules are attached on the edge C_3N nanoribbon.

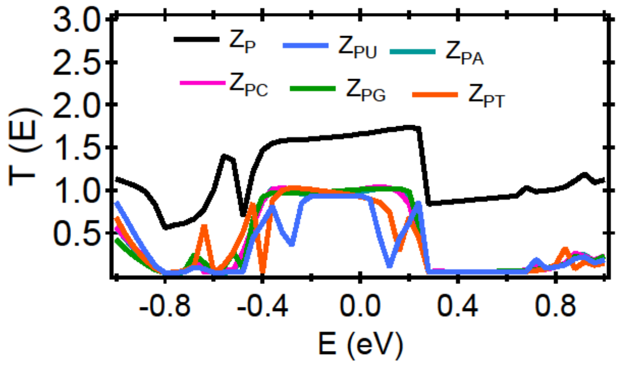

Fig.S2 The transmission coefficient as function of energy of DNA/RNA attached on Z_P.

B. Effect of Doping

To see the effect of doping on transport properties of C_3N, we took both p/n (boron/sulphur) type of doping elements at middle/edge locations on C_3N nanoribbon.

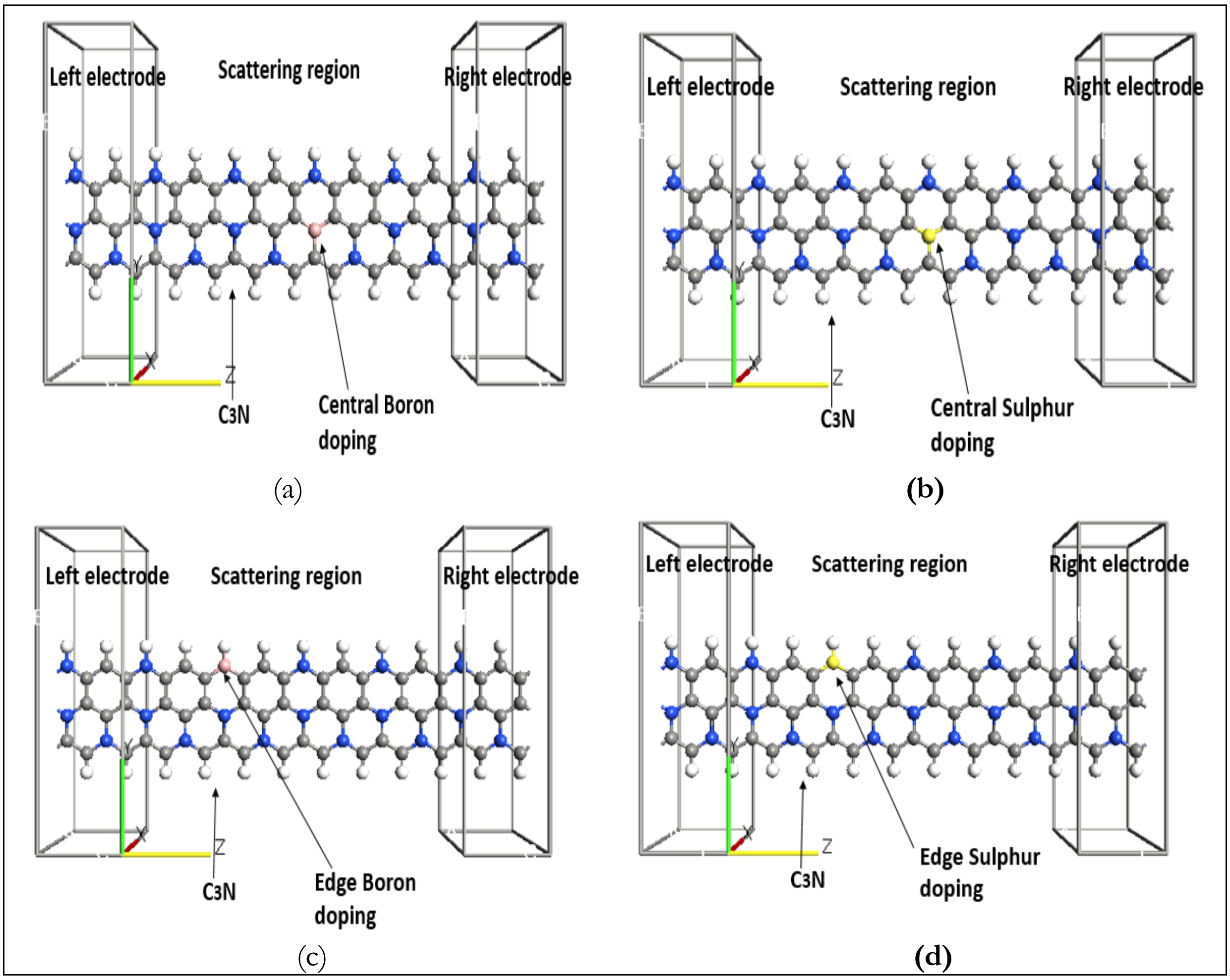

Fig. S3 (a)-(d) The schematic 2-probe geometry of boron and sulphur doping atoms at middle and edge locations on C_3N.

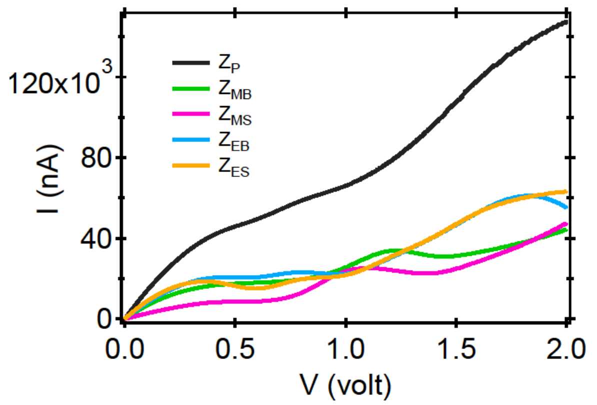

Fig. S4 The I-V characteristics of C_3N with boron/sulphur doping at middle and edge locations

C. Effect of concentration

To calculate the effect of concentration of DNA molecules on transport properties of C_3N, we have attached adenine molecules sequentially on both sides of C_3N nanoribbon.

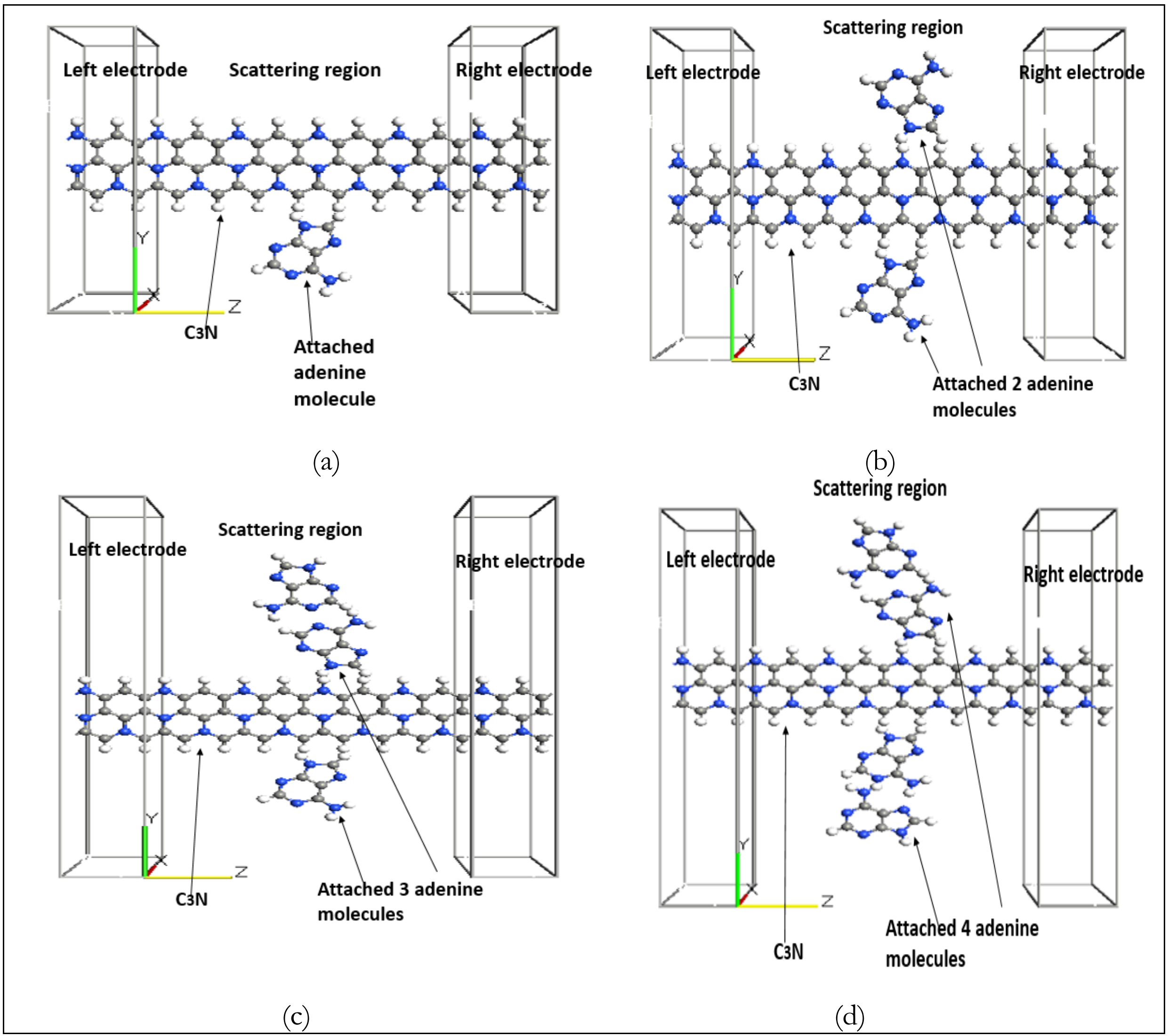

Fig.S5 (a)-(d) shows the schematic geometry of C_3N with different concentration of adenine molecules are attached on both sides of nanoribbon.

D. Effect of defect

Here, we studied DV, SV and SW defect in C_3N nanoribbon as shown below.

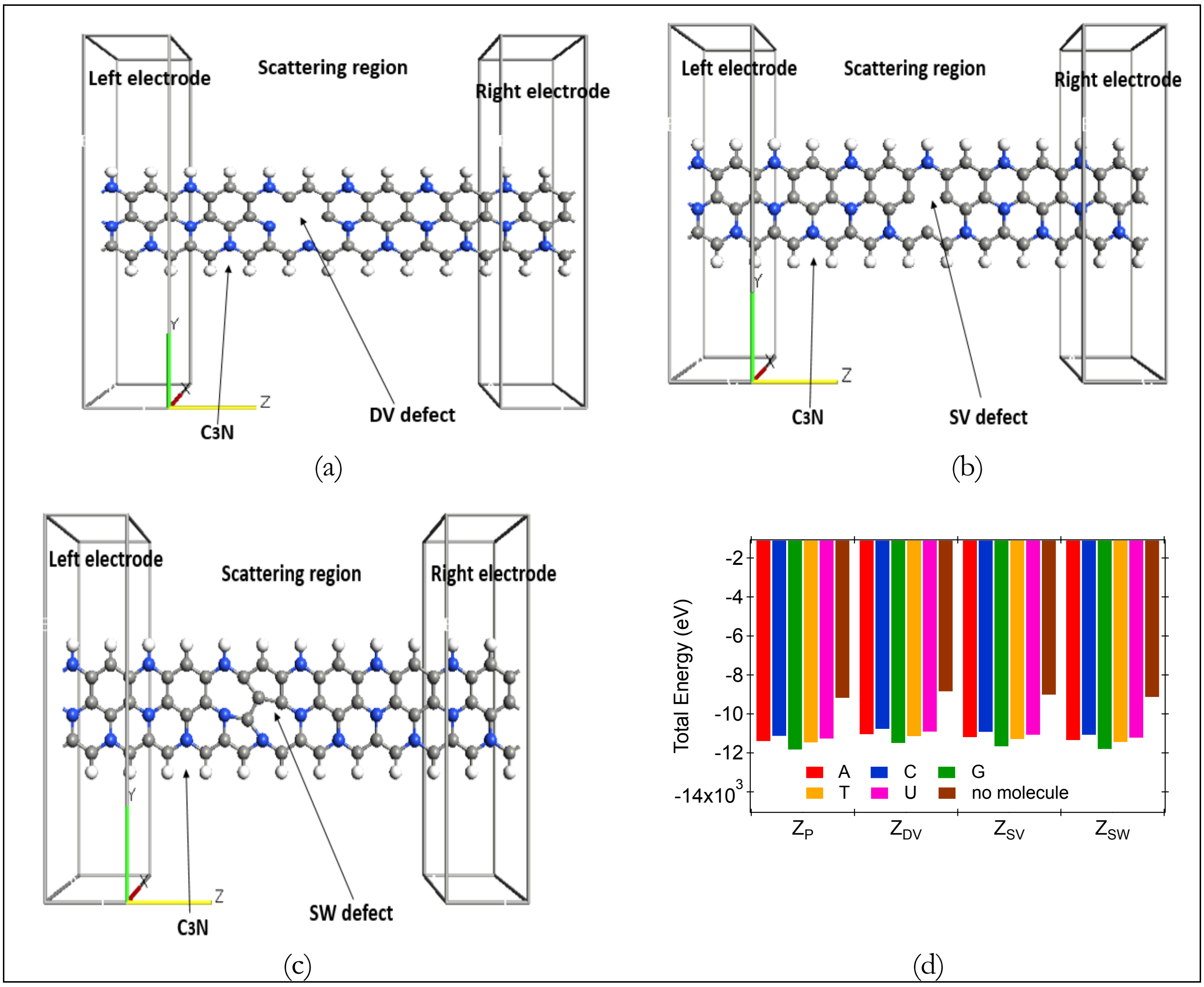

Fig.S6: The schematic 2-probe geometry of C_3N nanoribbon with (a) double vacancy, (b) single vacancy and (c) stone wales defect. (d) The variation in total energy of defective (SV, DV and SW) C_3N and DNA molecules attached with C_3N nanoribbon.

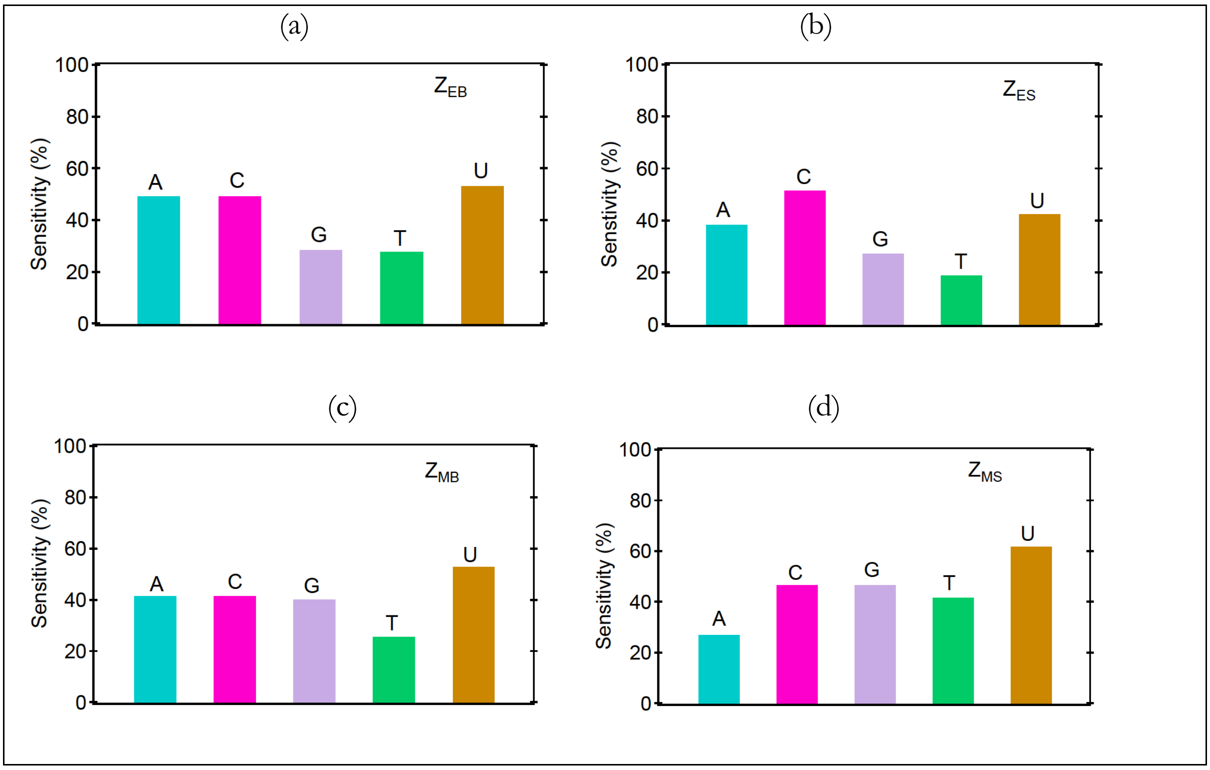

Fig. S7 Variation in the sensitivity of doped nanoribbon in the presence of DNA/RNA nucleobases.

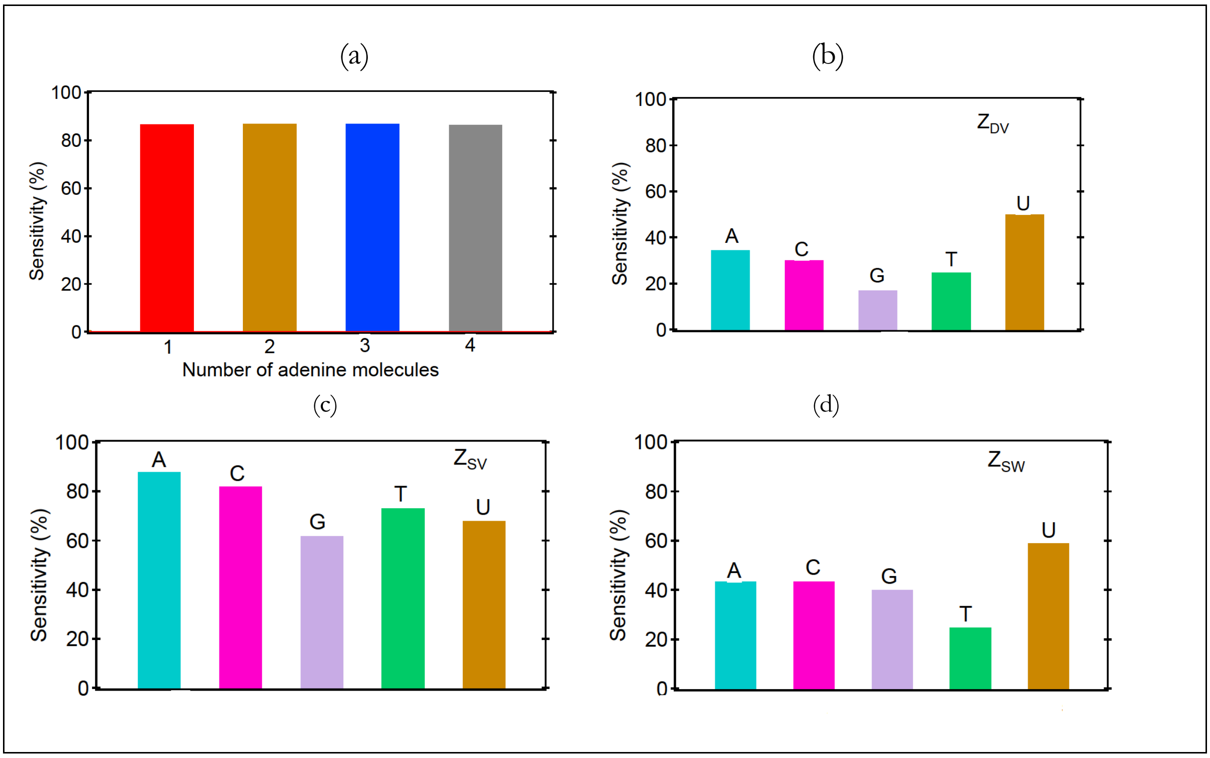

Fig. S8: Variation in the sensitivity of nanoribbon for (a) different concentration of adenine molecules (b) double vacancy (DV), (c) single vacancy (SV) and (d) stone wales (SW) defective nanoribbon in the presence of DNA/RNA nucleobases

E. Adsorption Energy of the nucleobases

The adsorption/binding energy of a nucleobase can be defined as, $E_a = E_{layer} - E_{molecule} - E_{layer+molecule}$. The adsorption energy (E_a) of the nucleobases vary between 1 - 1.35 eV on the pristine system with, G highest and C with lowest binding strength. Independent of the dopant type, the location of the dopant atom has a larger impact on the E_a. Doping at the centre of nanoribbon with B or S atom resulted in an increase in E_a with maximum change for U. On the other hand, edge doping leads to a significant reduction in E_a and the value of E_a does not change between S and B doping. In the presence of a vacancy, E_a is highest for single vacancy (SV) case and lowest for stoner-wales (SW) defect with the maximum E_a for U in all three cases.

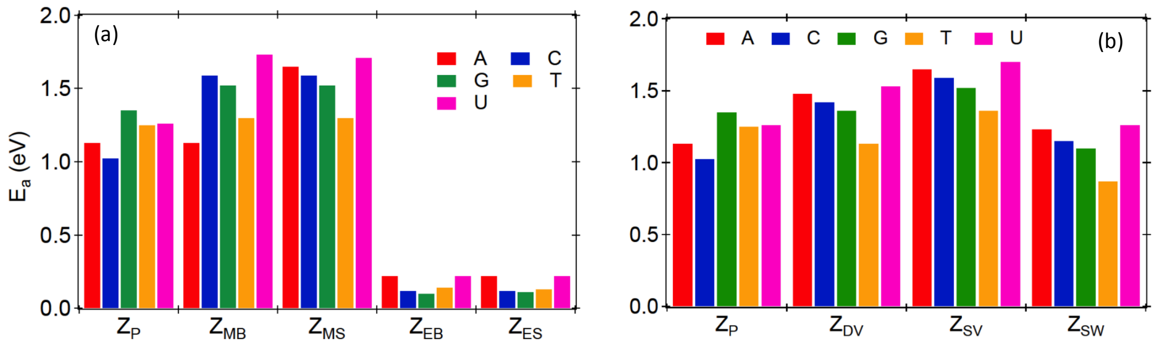

Fig. S9: Variations in binding energy of DNA/RNA nucleobase in different (a) doping and (b) defect configurations of C_3N nanoribbon.

F. Effect of Gate Voltage on Transmission Spectrum

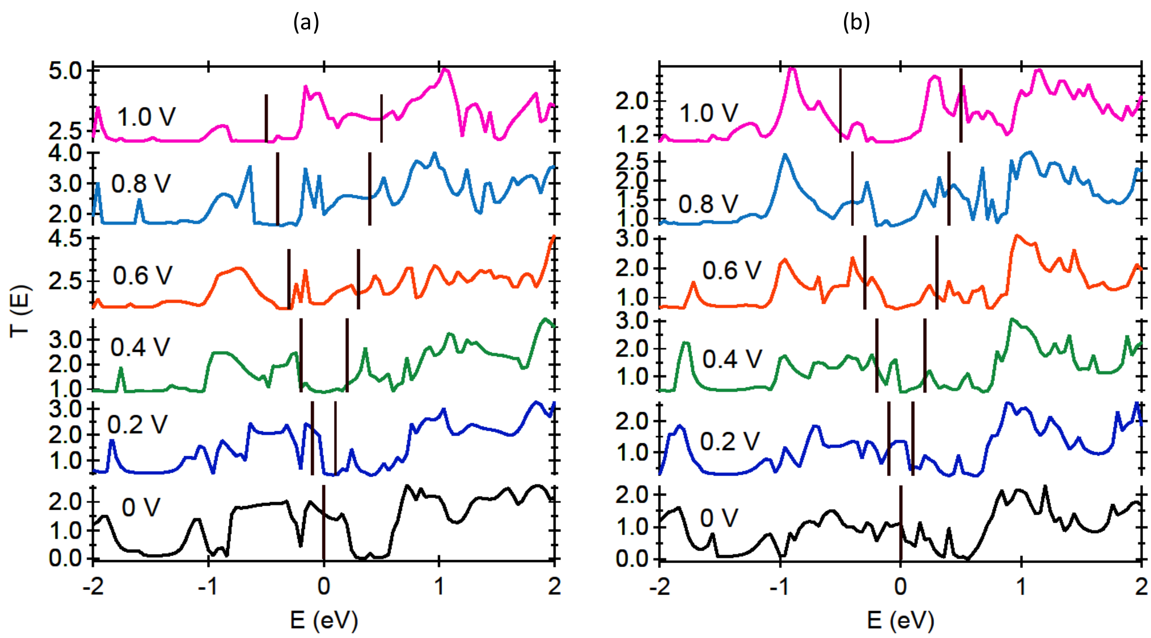

Fig. S10: Transmission spectrum of (a) Z_P and (b) Z_{PA} at V_g = 10 V in the FET geometry.

G. Effect of doping and defect on Transmission Spectrum

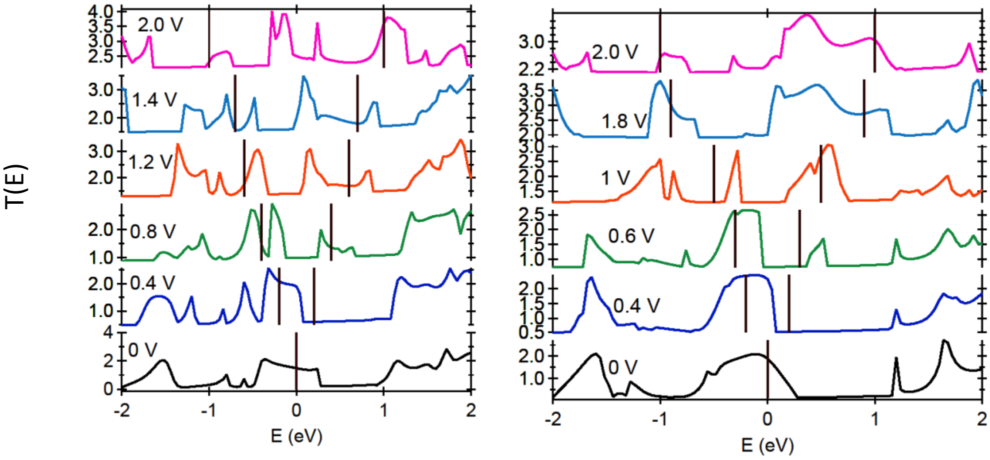

Fig. S11: The transmission spectrum of (left) Z_{MB} and (right) Z_{EB} at different applied voltages.

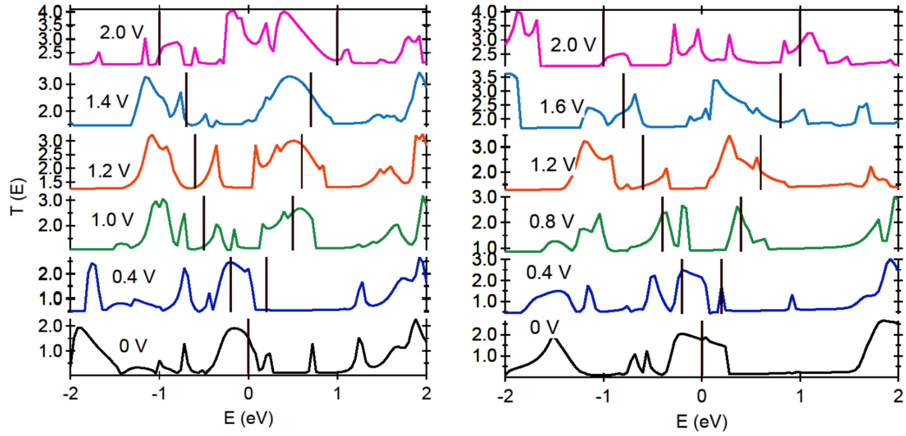

Fig. S12: The transmission spectrum of (left) Z_{DV} and (right) Z_{SV} at different applied voltages.