

Supplementary information

P-type doping in edge-enriched MoS_{2-x} nanostructure via RF-generated nitrogen plasma

Khomdram Bijoykumar Singh^{a,b}, Jyotisman Bora^a, Bablu Basumatary^{a,c}, Shakyadeep Bora^{a,b}, and Arup Ratan Pal ^{*a,b}

^aPlasma Nanotechnology Laboratory, Institute of Advanced Study in Science and Technology, Guwahati (IASST), Guwahati-781035, India

^bAcademy of Scientific and Innovative Research (AcSIR), Ghaziabad – 201002, India

^cDepartment of Metallurgical Engineering and Materials Science, Indian Institute of Technology Bombay, Mumbai-400076, India

*Corresponding author email: arpal@iasst.gov.in

List of figures and tables

Figure S1: FESEM images of MS, MS5 and MS10 taken at low magnification..	2
Figure S2: RMS roughness distribution graph of MS, MS5 and MS10.....	2
Figure S3: EDX spectra recorded at HRTEM for MS,MS5 and MS10..	3
Figure S4: FESEM image of v-MS on carbon-coated copper TEM grid.....	4
Figure S5: XPS survey spectra of MS, MS5 and MS10.....	4
Figure S6 represents the content of different elements in MS, MS5, and MS10..	4
Figure S7: (a) Uv-Vis absorbance spectra (b) Tauc plot of MS,MS5 and MS10.....	5
Figure S8: OES spectra for N ₂ plasma at RF power 5W and 10W for actinometry method.....	5
Table T1 illustrates the variation of Mo-N bond due to plasma treatment...	3
Table T2: Calculated value of work function and valence band position..	3
Vander Pauw method for finding conductivity type and carrier density.....	5

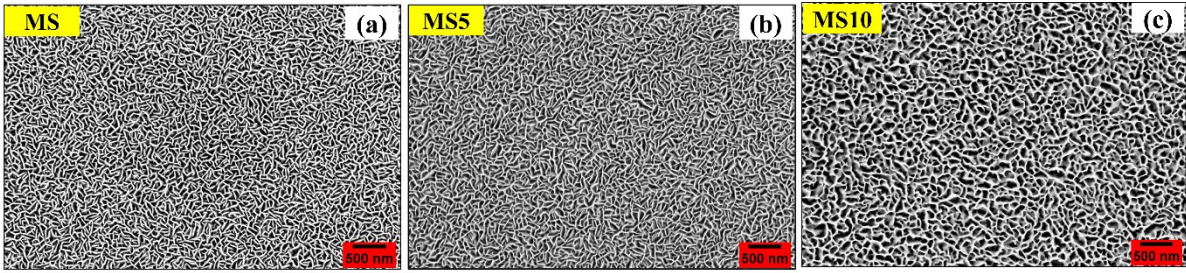


Figure S1: FESEM images of (a) MS (b) MS5 and (c) MS10 taken at low magnification. It clearly shows that the nanostructure is deposited uniformly.

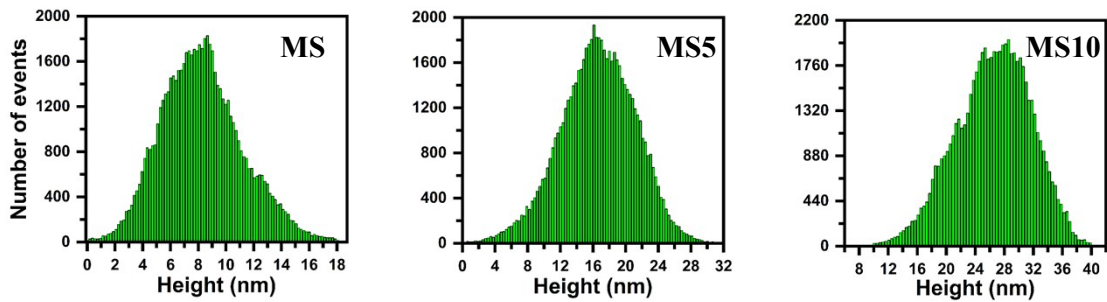


Figure S2: RMS roughness distribution graph of MS, MS5 and MS10 from KPFM surface topography images. Average RMS roughness of MS, MS5 and MS10 is 3.954 ± 0.09 nm, 3.973 ± 0.574 nm and 5.283 ± 0.183 nm respectively. Roughness increases with plasma treatment.

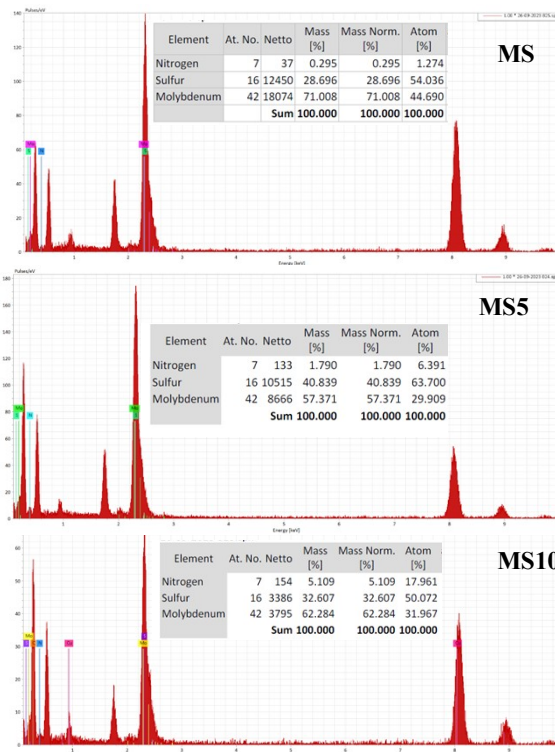


Figure S 3: EDX spectra recorded at HRTEM for MS,MS5 and MS10. It shows the increment of N content with plasma treatment.

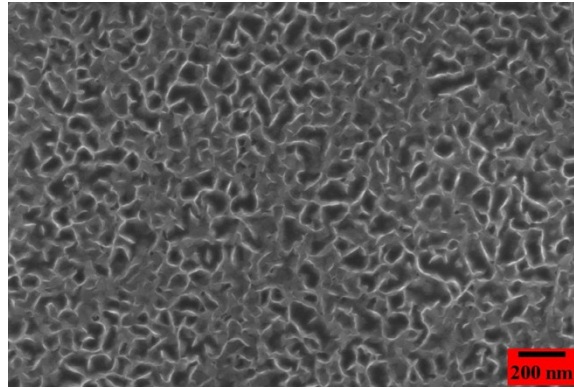


Figure S4: FESEM image of v-MS on carbon-coated copper TEM grid. It shows that the vertically oriented nanostructure is independent of the substrate.

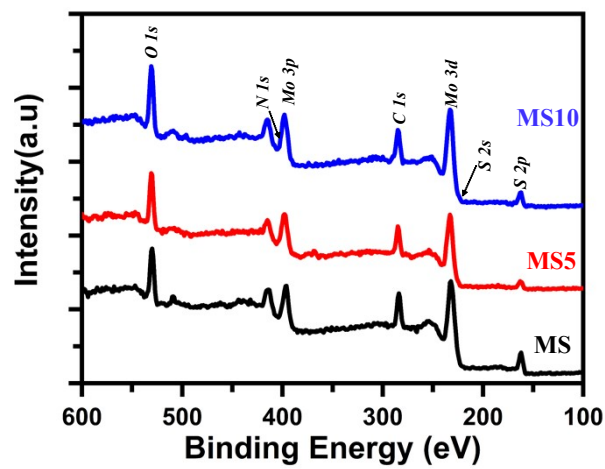


Figure S5: XPS survey spectra of MS, MS5 and MS10. It indicates the presence of Mo, S, N, O and C and their content are summarised in the following graph.

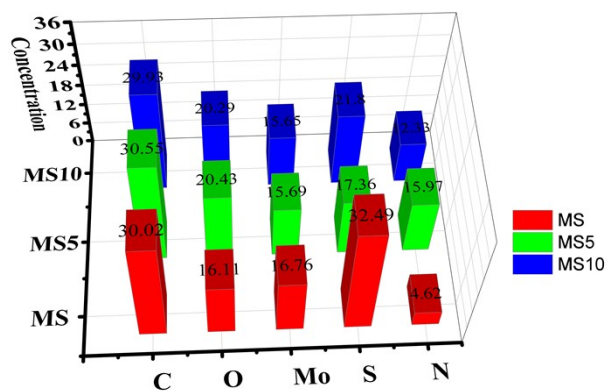


Figure S6 represents the content of different elements in MS, MS5, and MS10. It shows that there is an increase in nitrogen content as sulfur content decreases.

Table T1 illustrates the variation of Mo-N bond due to plasma treatment. Mo-N abruptly increases showing the the substitution of S.

Samples	Mo-S	Mo-N	Pyridic N
MS	1	0.15	0.05
MS 5	1	1.73	0.26
MS 10	1	1.25	0.03

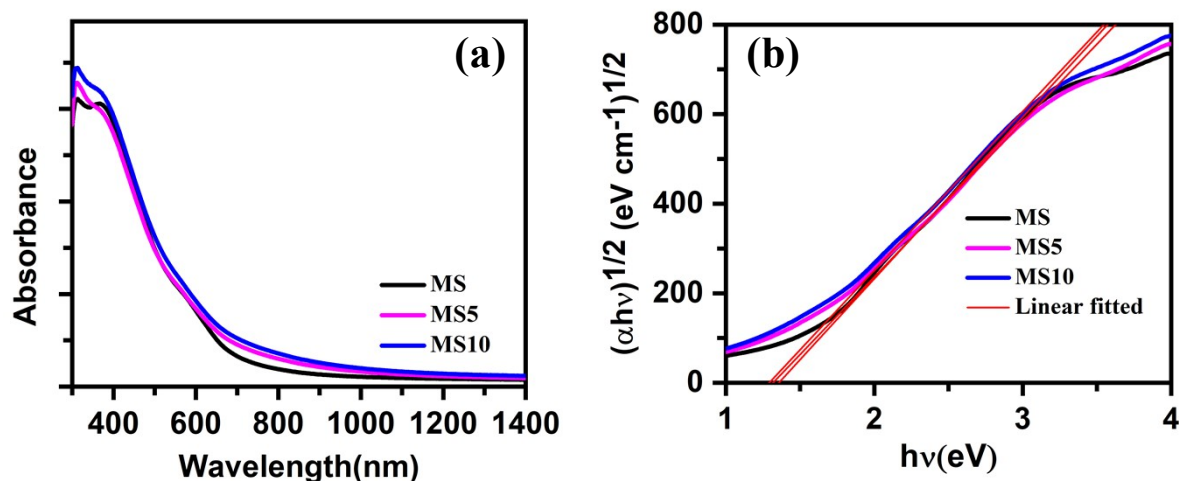


Figure S7: (a) UV-Vis absorbance spectra (b) Tauc's plot of MS,MS5 and MS10. Considering the indirect band gap, the band gap for MS, MS5, and MS10 is found to be 1.35 ± 0.01 eV, 1.31 ± 0.01 eV. For indirect band gap, $\alpha hv = (hv - E_g)^2$ relation is used to find the band gap of the material.

Table T2: Calculated value of work function and valence band position. E_{SE} and E_{FE} are calculated

Sample	E_{SE} (eV)	E_{FE} (eV)	Work function (eV)	Valence band position (eV)
MS	4.02	20.39	4.83	5.72
MS5	4.02	21.07	4.15	4.55
MS10	4.02	21.14	4.08	4.39

from the results obtained in Figure 5 (a) & (b).

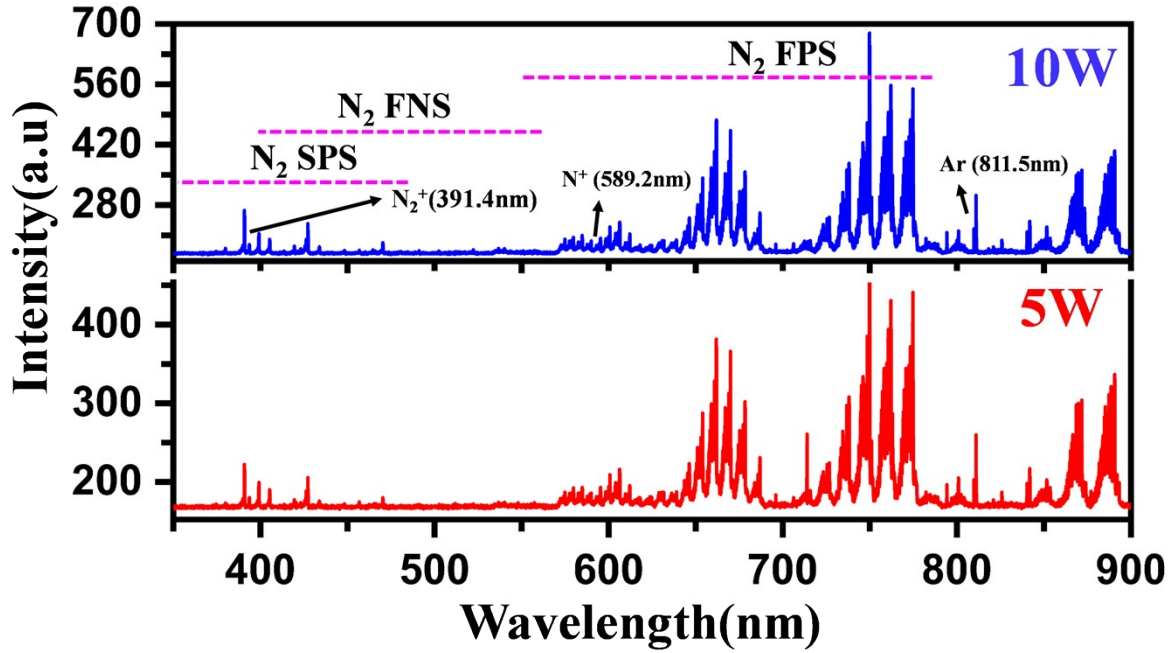


Figure S8: OES spectra for N₂ plasma at RF power 5 W and 10 W for actinometry method. 5% argon gas of total pressure is used for actinometry method. Argon line at 811.5 nm is used for relative quantification of N⁺(589.2 nm) and N₂⁺(391.4 nm).

Van der Pauw Method for finding conductivity type and carrier density

To confirm the conductivity type, Van der Pauw method is used. A magnetic field of strength 0.35 T is used. Hall coefficient is given by the formula

$$R_H = \left(\frac{t}{I \cdot B}\right) \frac{1}{4} [(V_{H1} - V_{H2}) - (V_{H1x} - V_{H2x})]$$

where t = thickness of the film ;

I= constant current applied

B = strength of the magnetic field in Tesla

V_{H1} = potential across 3 and 4 when current is applied from 1 to 2 with B upward

V_{H2} = potential across 3 and 4 when current is applied from 2 to 1 with B upward

V_{H1x} = potential across 3 and 4 when current is applied from 2 to 1 with B downward

V_{H2x} = potential across 3 and 4 when current is applied from 1 to 2 with B downward

Since $R_H = \frac{1}{n \cdot q}$, carrier concentration (either electrons or holes concentration) is given by $n = \frac{1}{R_H \cdot q}$ where $q = 1.6 \times 10^{-19} \text{ C}$.

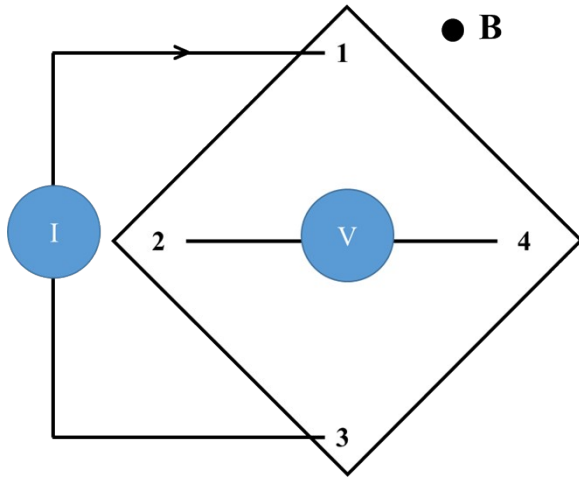


Figure S9: Circuit connection for Van der Pauw method

It is observed that the Hall coefficient for pristine sample (MS) is $-2.314 \text{ } \Omega \cdot \text{cm} \cdot \text{T}^{-1}$ while for plasma treated samples MS5 and MS10 it is $11.102 \text{ } \Omega \cdot \text{cm} \cdot \text{T}^{-1}$ and $701.201 \text{ } \Omega \cdot \text{cm} \cdot \text{T}^{-1}$ respectively. From the sign of the Hall coefficient, it can be concluded that upon plasma treatment, the n-type conductivity of MS changes to p-type conductivity. Also, the carrier density for MS (i.e. electrons) is $2.7 \times 10^{18} \text{ per cm}^3$ whereas those of MS5 and MS10 (i.e. holes) are $5.62 \times 10^{17} \text{ per cm}^3$ and $8.91 \times 10^{15} \text{ per cm}^3$ respectively.