

Electronic Supplementary Information

Dual role of g-C₃N₄/carbon intra Schottky junction in charge carrier generation and separation for efficient solar H₂ production.

A. R. Mahammed Shaheer^a, *P. Karthik*^a, *G. Karthik*^b, *M. V. Shankar*^c and *B. Neppolian*^{a*}

^a SRM Research Institute and Department of Chemistry, SRM Institute of Science and Technology, Kattankulathur, Chennai - 603203, Tamil Nadu, India.

^b Department of Nuclear Physics, University of Madras, Chennai – 600024, Tamil Nadu, India.

^c Nanocatalysis and Solar Fuels Research Laboratory, Department of Materials Science and Nanotechnology, Yogi Vemana University, Kadapa - 516005, Andhra Pradesh, India.

*neppolian.b@res.srmuniv.ac.in

Contents List

Section S1. Solar to hydrogen (STH) efficiency calculation

Figure S1. SEM images of C100.

Figure S2. SEM and EDAX of (a) and (b) g-C₃N₄, (b) and (c) C₃N₄-5C, (e) and (f) C100.

Figure S3. FTIR spectrum of C100.

Figure S4. Wide Scan XPS of g-C₃N₄ and C₃N₄-5C.

Figure S5. Nitrogen sorption isotherms of g-C₃N₄ and C₃N₄-5C

Table S1. Different bonding percentage of deconvoluted N1s XPS spectra of g-C₃N₄ and C₃N₄-5C

Table S2. Life time decay data.

Table S3. STH (%) of prepared photocatalysts.

Table S4. BET Specific surface area of g-C₃N₄ and C₃N₄-5C

Section S1. Solar to hydrogen (STH) efficiency calculation

The solar to hydrogen efficiency can be calculated by following mathematical expression

$$STH(\%) = \frac{\text{Energy of generated } H_2}{\text{Solar energy irradiating the solution}} \times 100 = \frac{E_{H_2}}{E_{Solar}} \times 100$$

$$E_{H_2} = (H_2 \text{ in mol/sec}) \times 232 \text{ kJ/mol}$$

$$E_{Solar} = P \times S \times t$$

Where, P= Irradiated solar energy in W/m²

S= Area of irradiation in m²

t= Irradiated time in sec

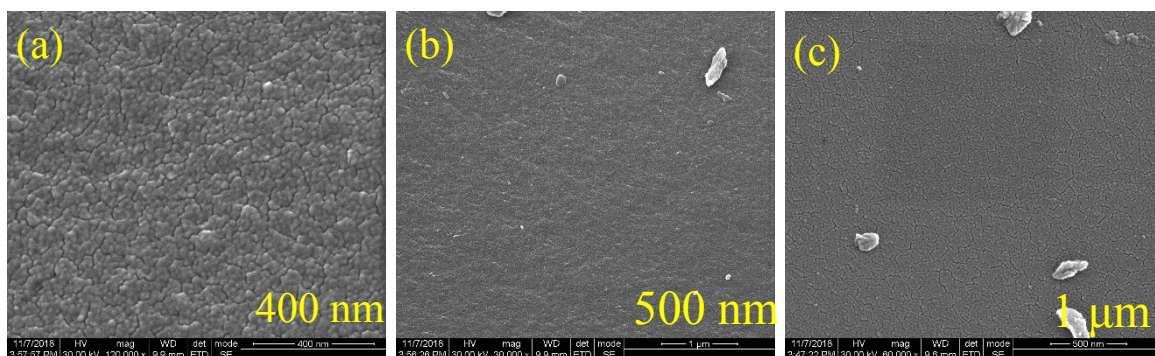


Figure S1. FE-SEM images of C100.

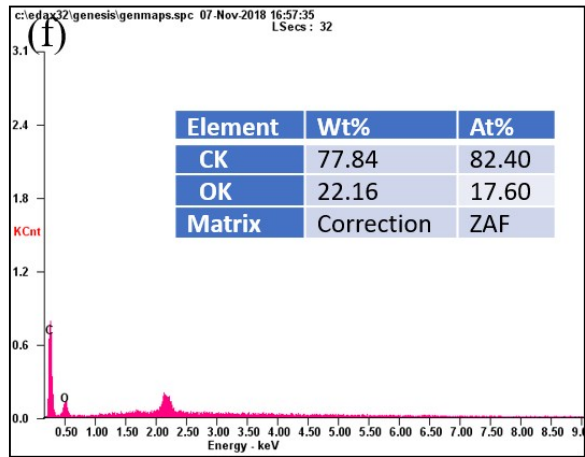
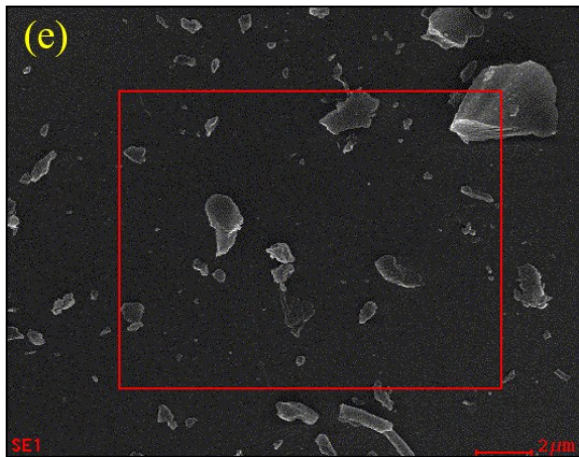
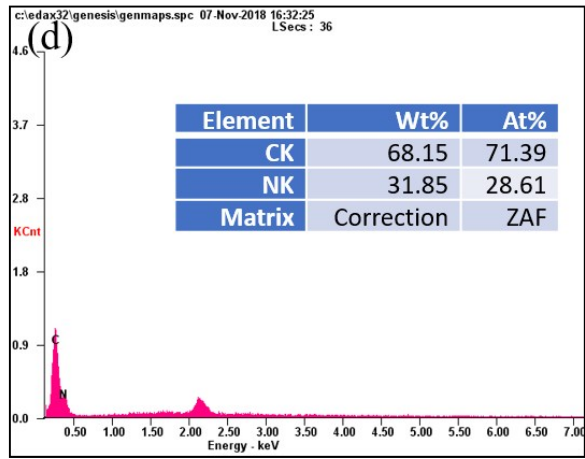
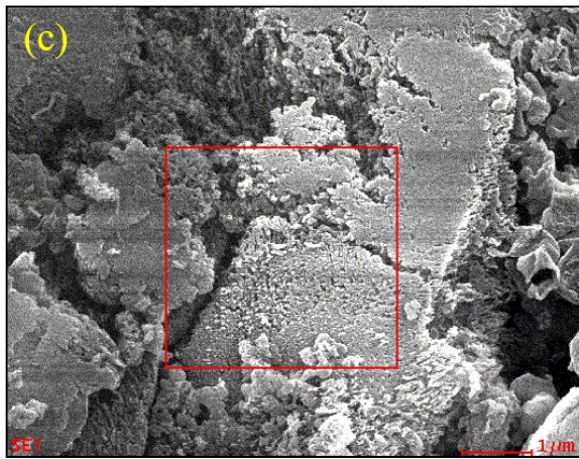
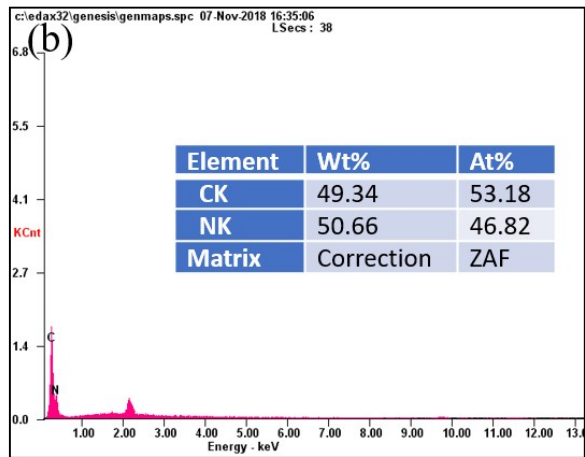
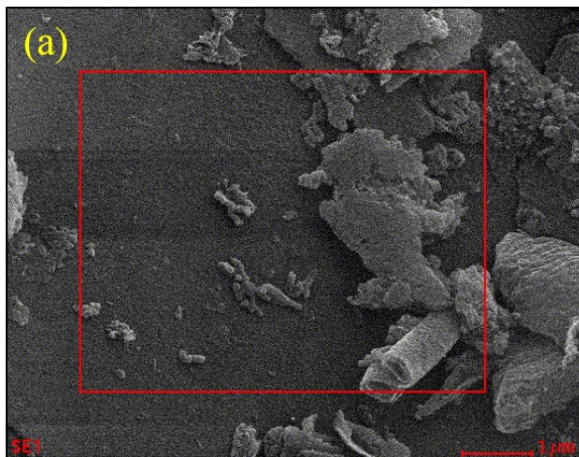


Figure S2. SEM and EDAX of (a) and (b) $g\text{-C}_3\text{N}_4$, (b) and (c) $\text{C}_3\text{N}_4\text{-5C}$, (e) and (f) C100 .

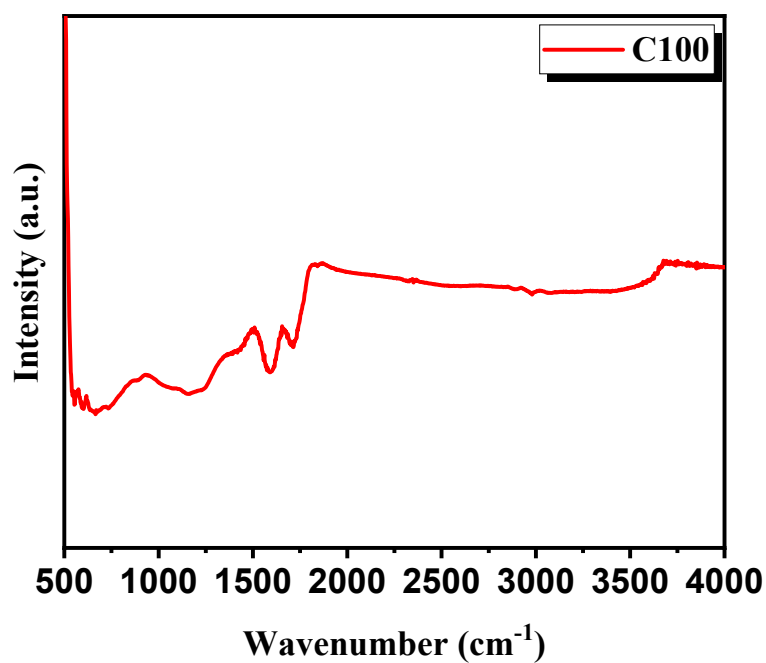


Figure S3. FTIR spectrum of C100.

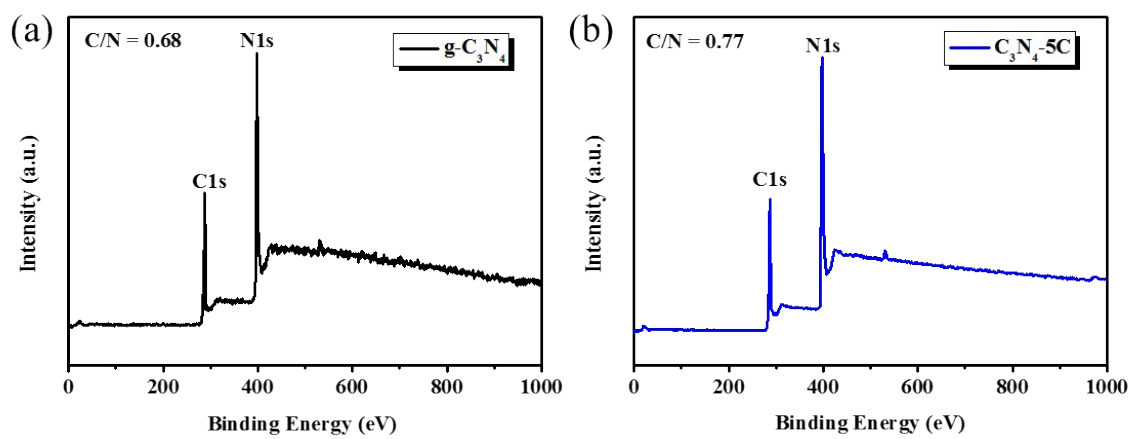


Figure S4. Wide Scan XPS of $g\text{-C}_3\text{N}_4$ and $\text{C}_3\text{N}_4\text{-5C}$.

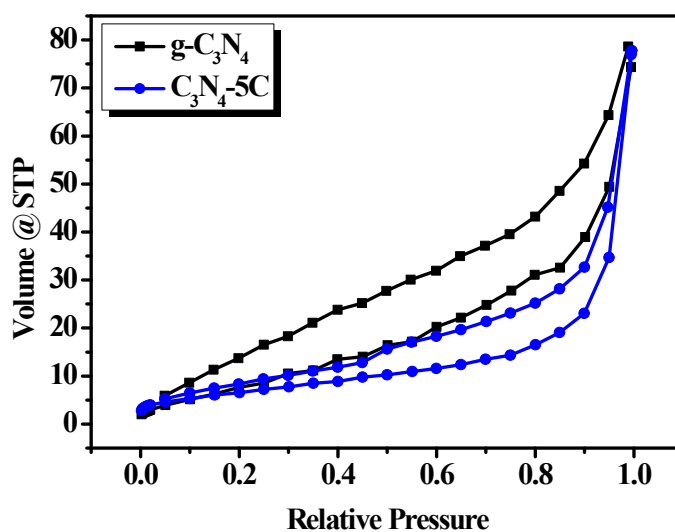


Figure S5. Nitrogen sorption isotherms of g-C₃N₄ and C₃N₄-5C

Table S1. Different bonding percentage of deconvoluted N1s XPS spectra of g-C₃N₄ and C₃N₄-5C

Sample Name	C=N-C	N-(C) ₃	C=N-H
g-C ₃ N ₄	0.52	0.33	0.15
C ₃ N ₄ -5C	0.48	0.41	0.11

Table S2. Life time decay data.

Sample	A1 (%)	η1 (ns)	A2 (%)	η2 (ns)	A3 (%)	η3 (ns)
C ₃ N ₄	16.6	2.24	83	11.2	0.4	0.047
C ₃ N ₄ -5C	16.6	1.34	0.4	0.031	83	6.63

Table S3. STH (%) of prepared photocatalysts.

Catalyst Name	STH (%)
C ₃ N ₄	0.015614
C ₃ N ₄ -2.5C	0.036531

C ₃ N ₄ -5C	0.102614
C ₃ N ₄ -7.5C	0.020781
C ₃ N ₄ -10C	0.007835
C100	0

Table S4. BET Specific surface area of g-C₃N₄ and C₃N₄-5C

Sample name	Surface Area (m²/g)	Pore Volume (cm³/g)
g-C ₃ N ₄	26.313	0.117
C ₃ N ₄ -5C	19.545	0.115