

Supporting Information for

# **Plasmon Assisted Highly Efficient Visible Light Catalytic CO<sub>2</sub> Reduction Over the Noble Metal Decorated Sr-Incorporated g-C<sub>3</sub>N<sub>4</sub>**

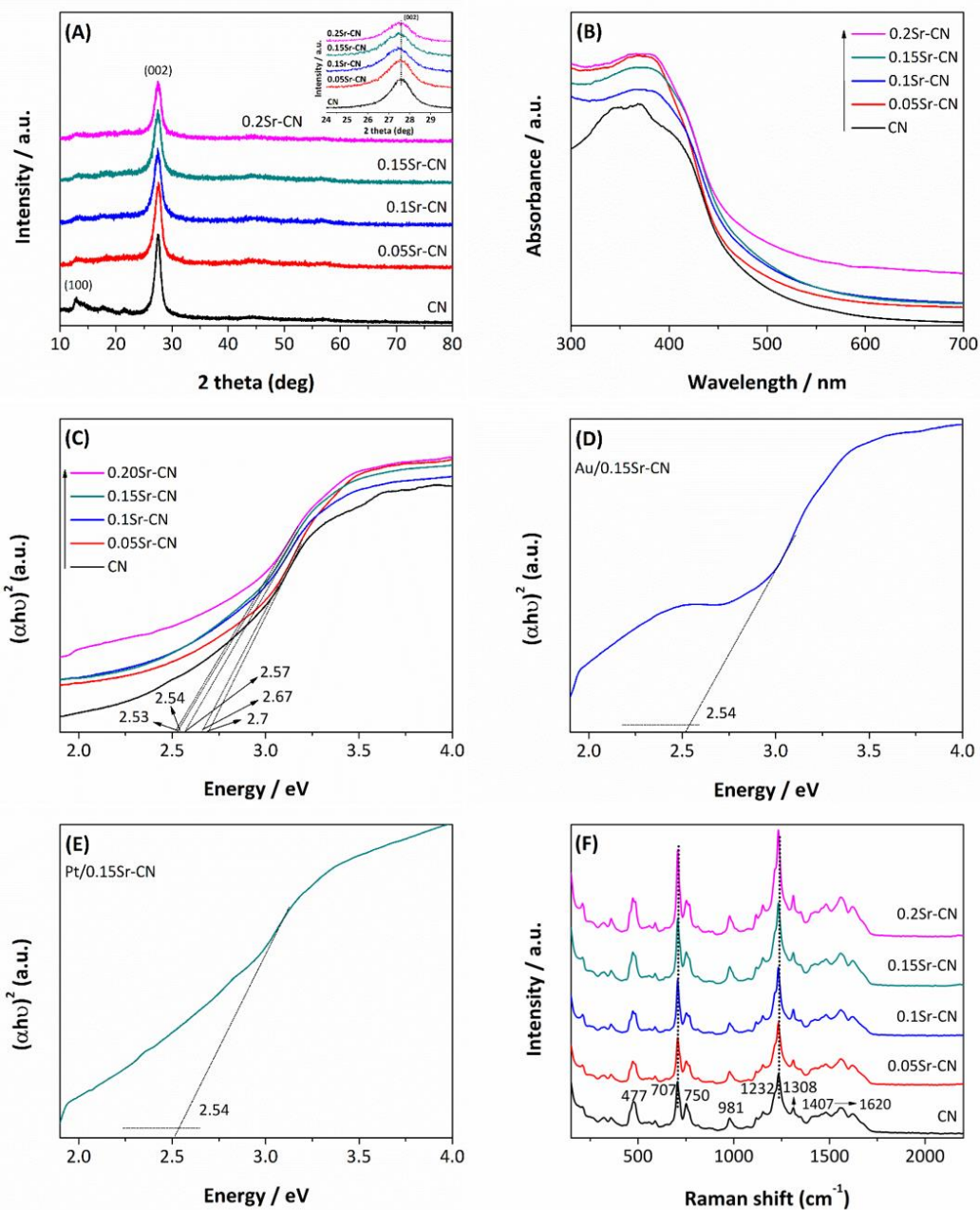
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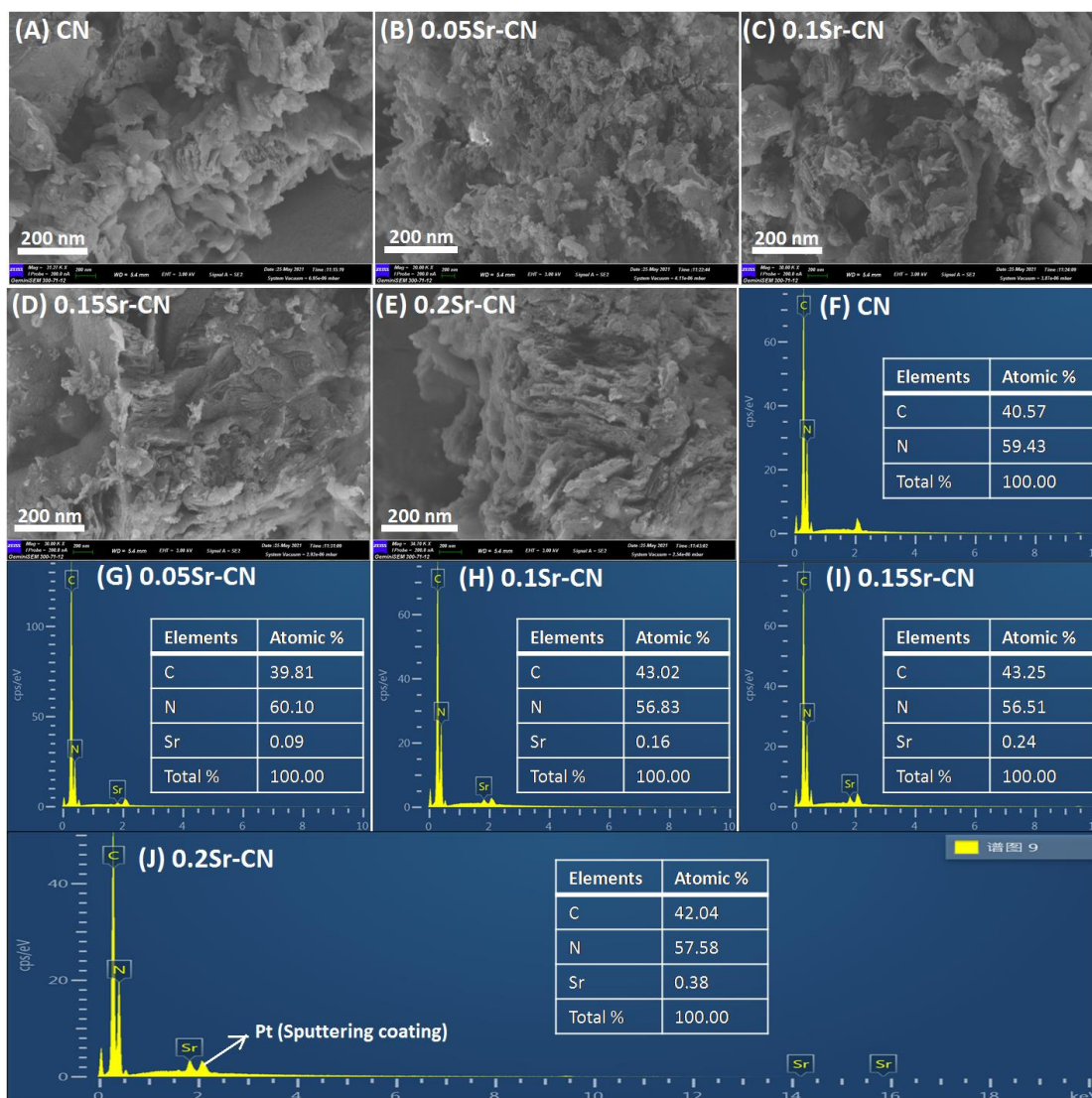
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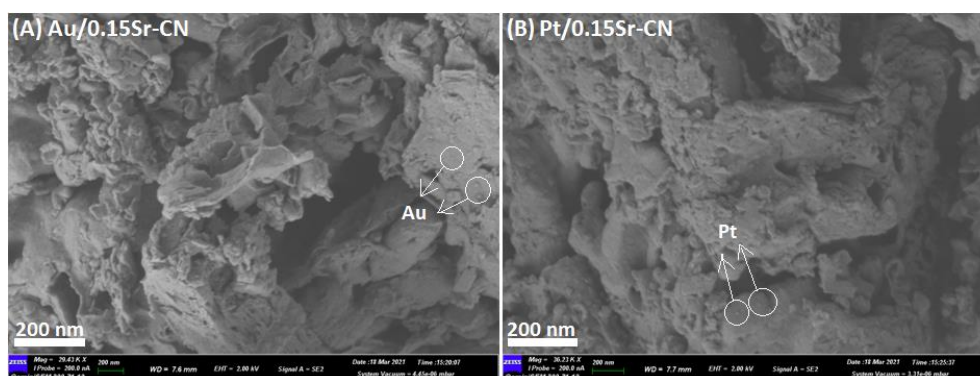
## Supplementary Figures and Tables



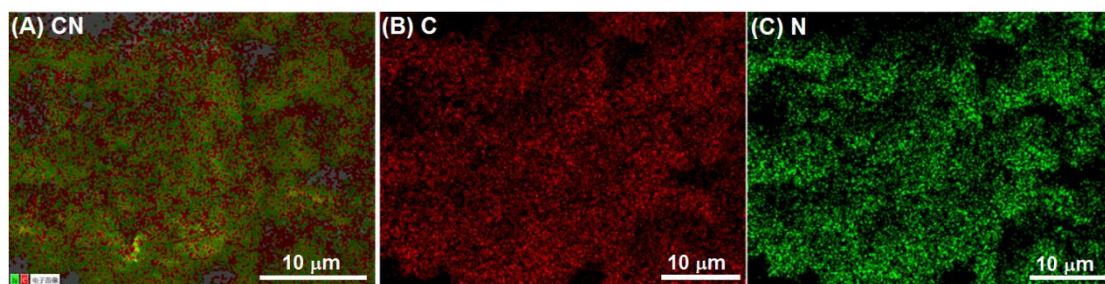
**Fig. S1** XRD patterns (a), UV-vis absorption spectra (b) and the calculated energy band gaps (c) of CN and  $x$ Sr-CN samples. Calculated energy band gaps (d) of Au/0.15Sr-CN and (e) of Pt/0.15Sr-CN sample. Raman spectra of the CN and  $x$ Sr-CN samples (f)



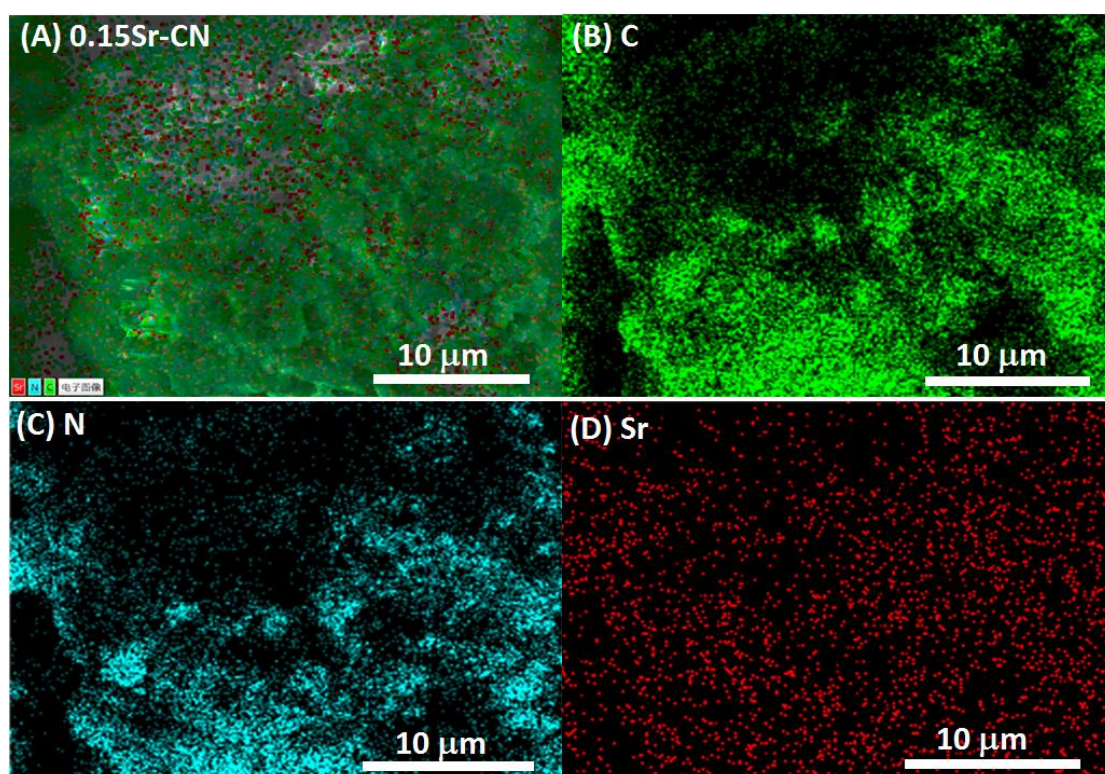
**Fig. S2** Scanning electron microscopy (SEM) micrographs (a) of CN, (b) of 0.05Sr-CN, (c) of 0.1Sr-CN, (d) of 0.15Sr-CN and (e) of 0.2Sr-CN. Energy dispersive X-ray spectroscopy (EDX) spectra: (f) of CN, (g) of 0.05Sr-CN, (h) of 0.1Sr-CN, (i) of 0.15Sr-CN and (j) of 0.2Sr-CN samples with atomic percentage of each element as inset



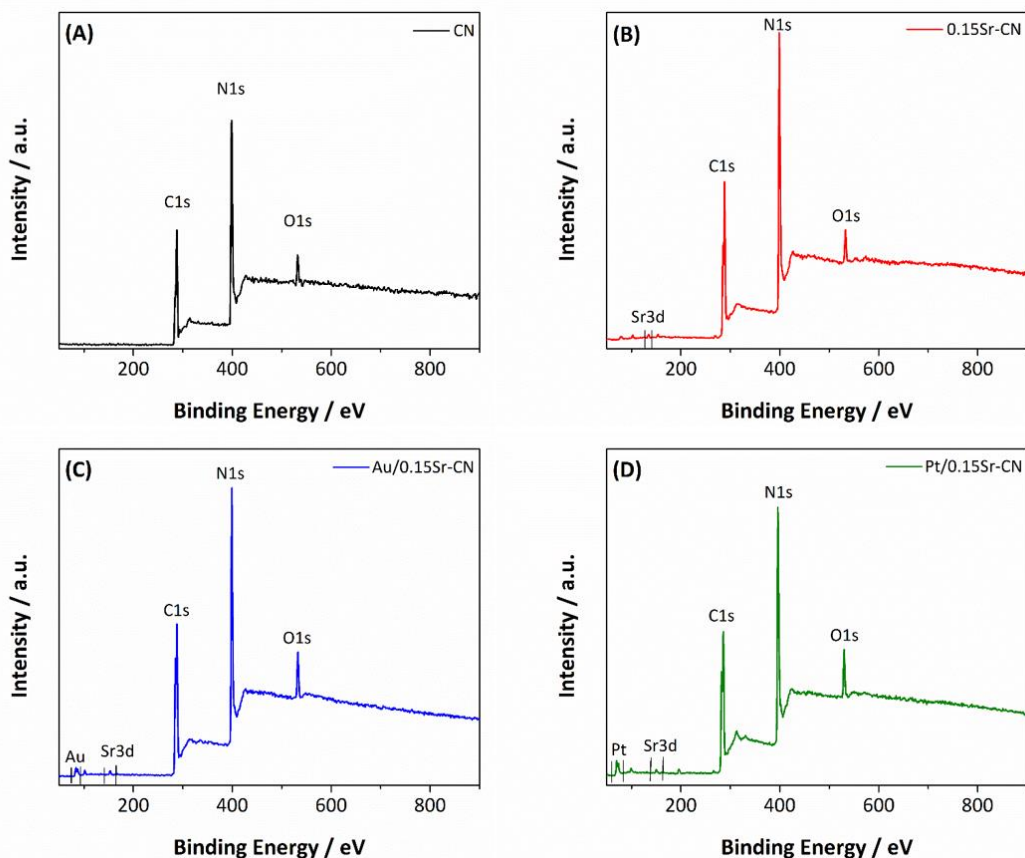
**Fig. S3** SEM micrographs; (a) of Au/0.15Sr-CN, and (b) of Pt/0.15Sr-CN samples



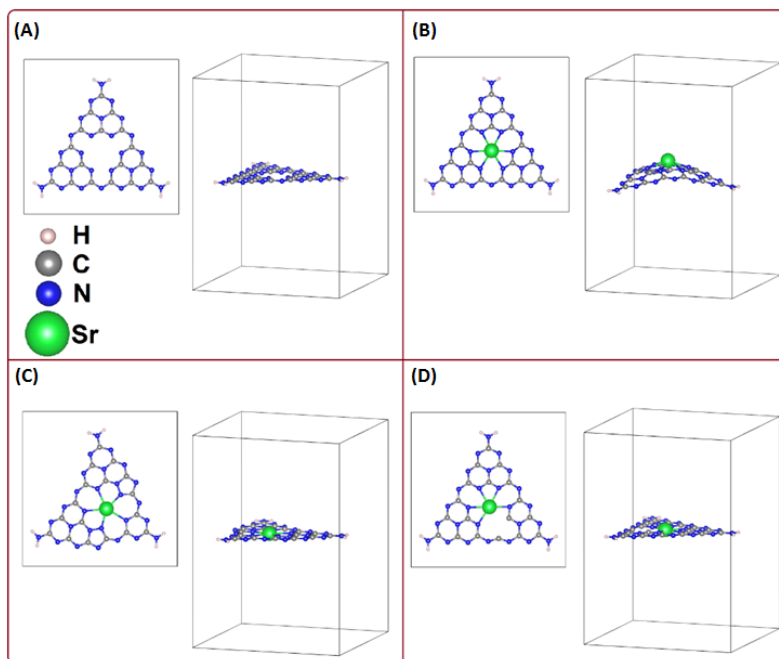
**Fig. S4** Energy Dispersive X-ray Spectra (EDS) mappings of (a) CN, (b) C element and (c) N element



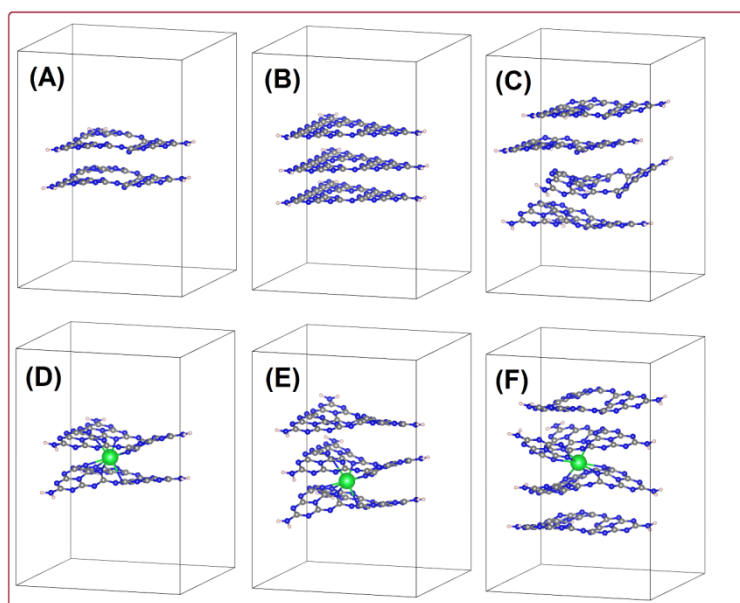
**Fig. S5** Energy Dispersive X-ray Spectra (EDS) mappings of (a) 0.15Sr-CN, (b) C element, (c) N element and (d) Sr element



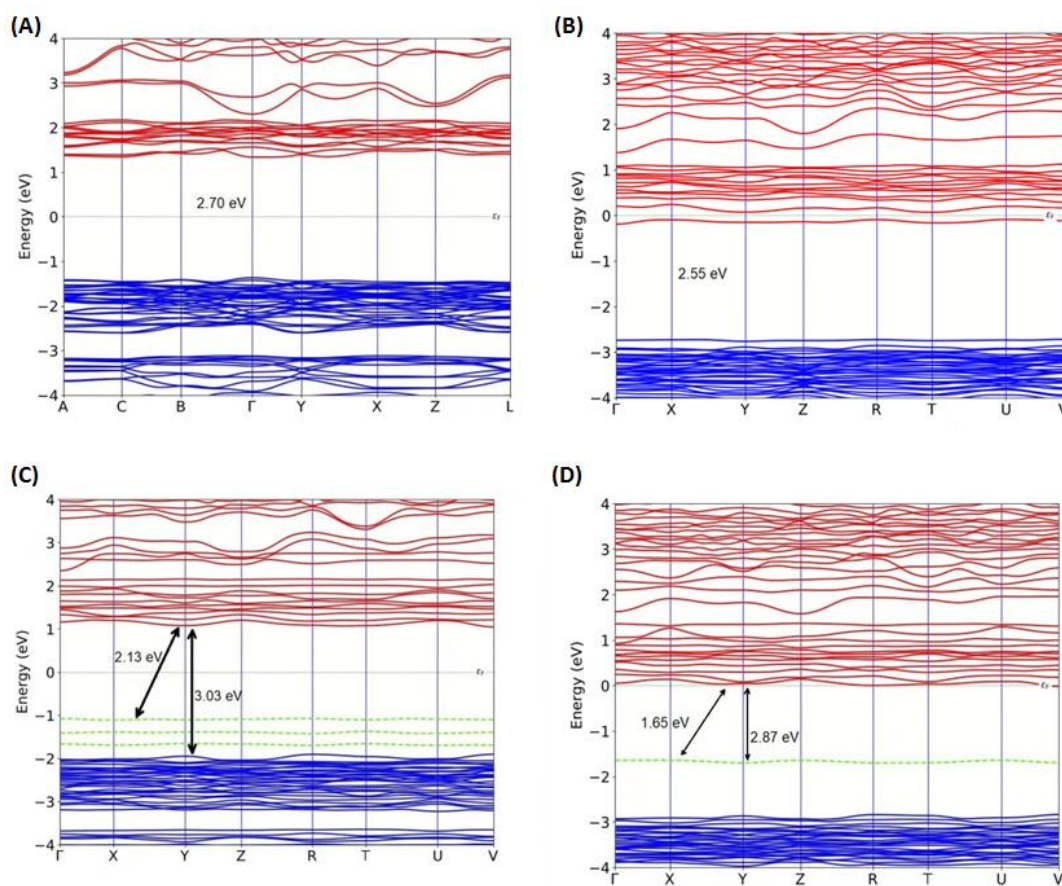
**Fig. S6** XPS survey spectra (a) of CN, (b) of 0.15Sr-CN, (c) of Au/0.15Sr-CN and (d) of Pt/0.15Sr-CN



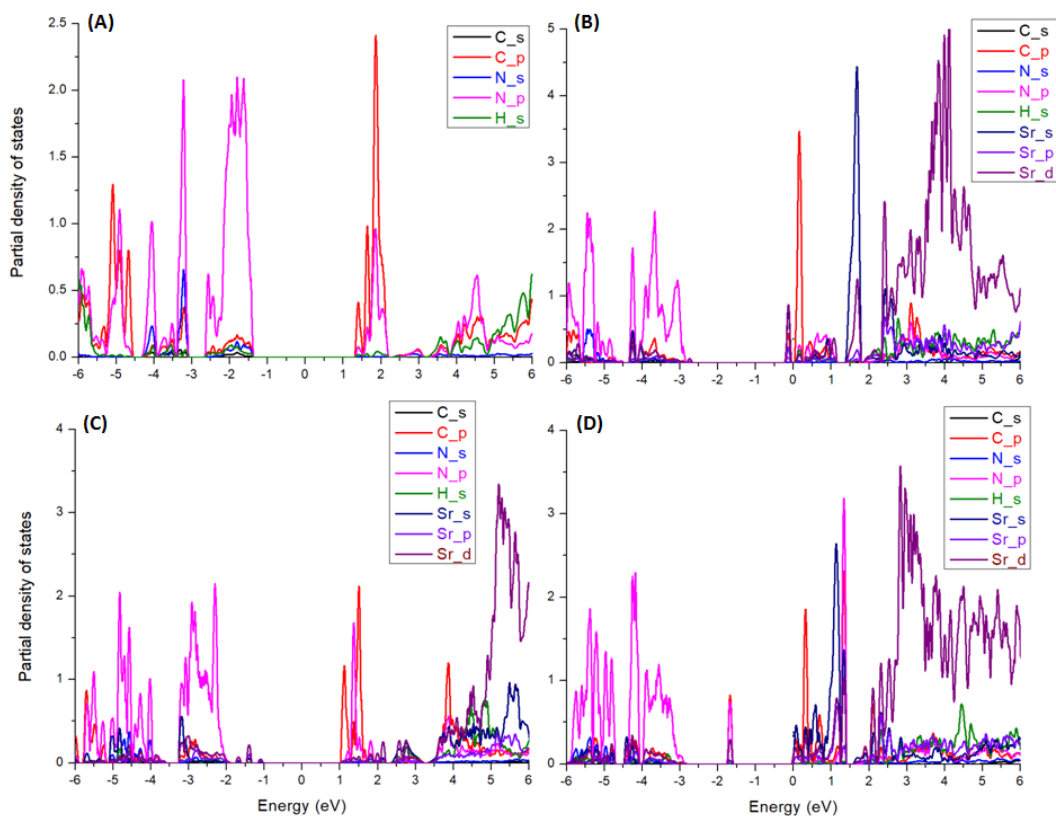
**Fig. S7** Optimized relaxed structure of CN (a), 0.15Sr-CN (Interstitial site) doping (b), 0.15Sr-CN (C-substituted) doping (c), and 0.15Sr-CN (N-substituted) doping (d)



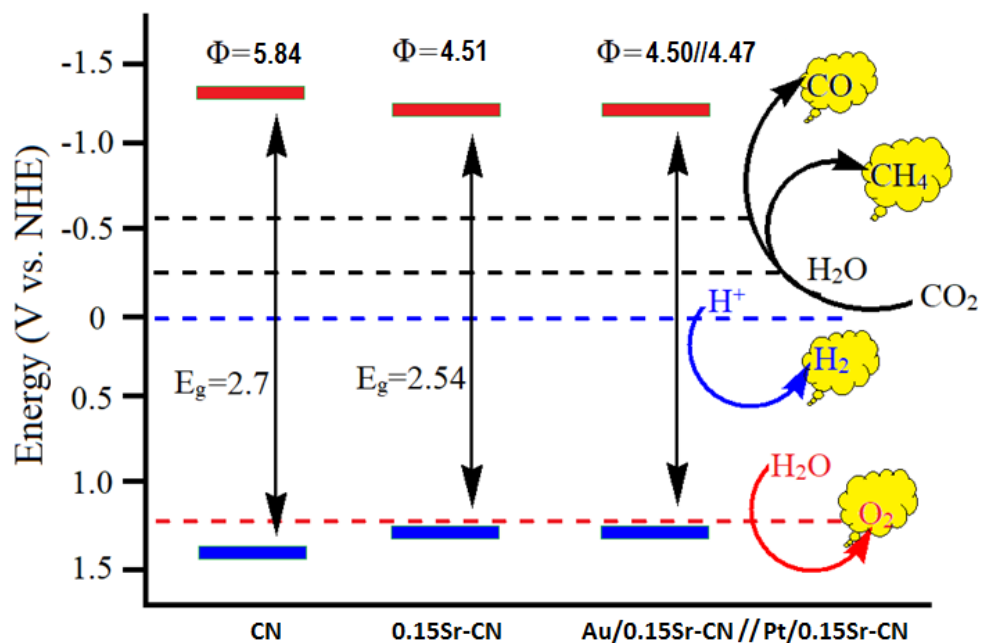
**Fig. S8** The optimized relaxed structure of two layers (a), three layers (b), four layers (c), and Sr-incorporated two layers (d), Sr-incorporated three layers (e), and Sr-incorporated four layers of CN (f)



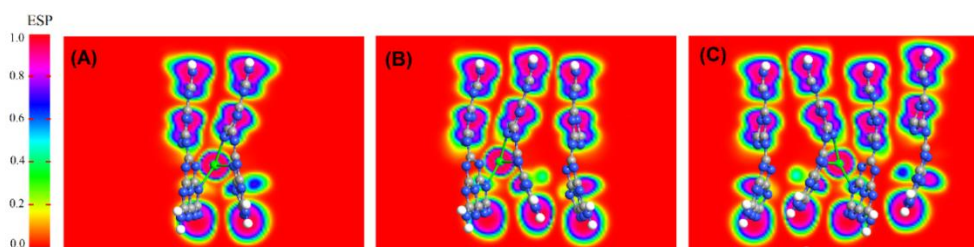
**Fig. S9** DFT calculated band structures of CN (a), of 0.15Sr-CN (Interstitial site) doping (b), of 0.15Sr-CN (C-substituted) doping (c), and of 0.15Sr-CN (N-substituted) doping (d)



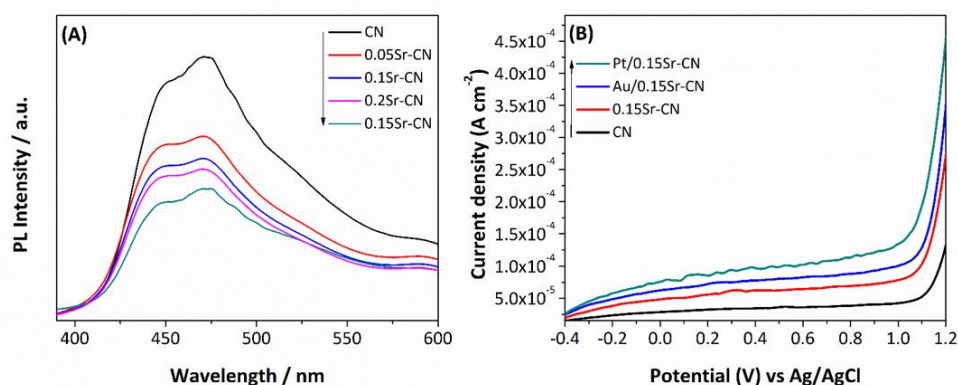
**Fig. S10** PDOS plots of pristine CN (a), 0.15Sr-CN (Interstitial site) doping (b), 0.15Sr-CN (C-substituted) doping (c), and 0.15Sr-CN (N-substituted) doping (d)



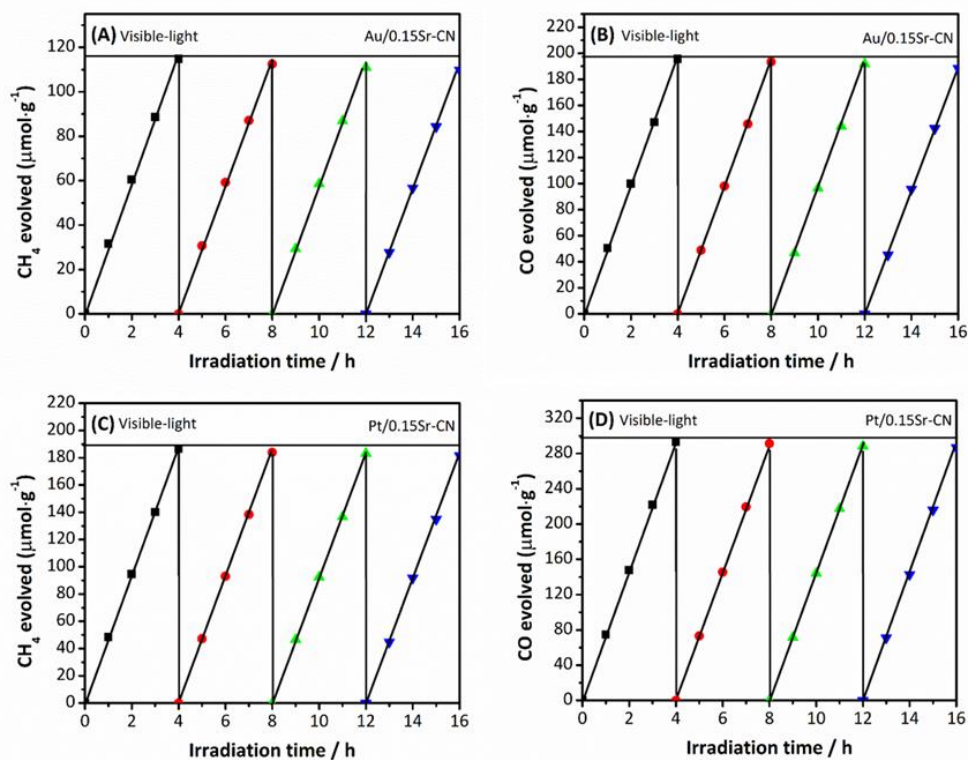
**Fig. S11** Energy band diagrams of the pristine CN, 0.15Sr-CN (interstitial), and Pt and Au deposited 0.15Sr-CN



**Fig. S12** Average electron density difference map for Sr-incorporated two layers (a), three layers (b), and four layers of CN (c)

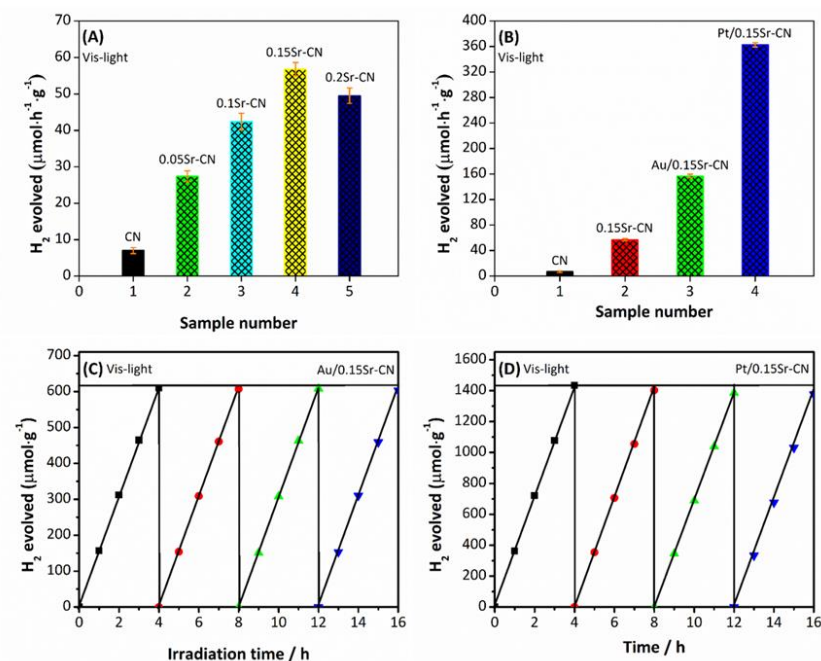


**Fig. S13** Photoluminescence (PL) spectra of CN and  $x$ Sr-CN samples (a), and photoelectrochemical  $I-V$  curves of CN, 0.15Sr-CN, Au/0.15Sr-CN and Pt/0.15Sr-CN samples (b)

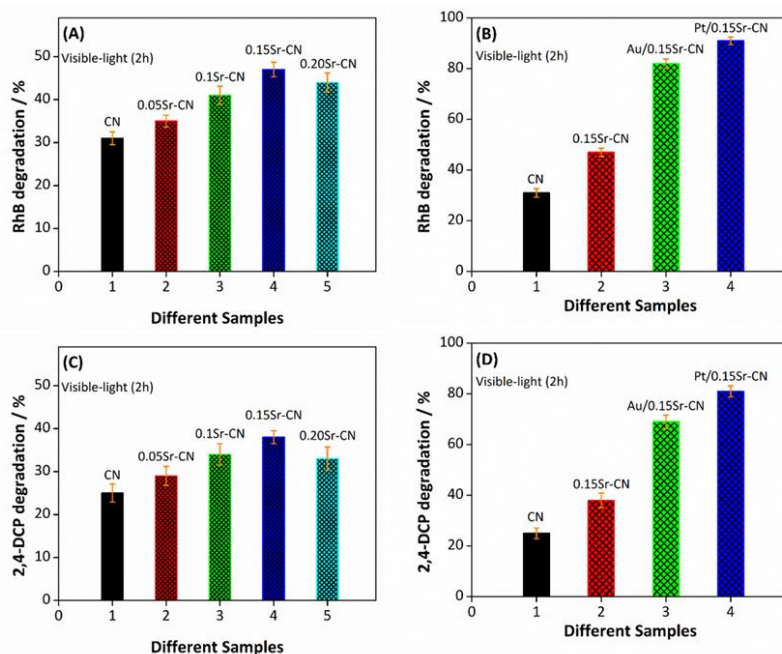


**Fig. S14** Photocatalytic recyclable tests for  $CO_2$  conversion to  $CH_4$  and CO products (a, b) over the Au/0.15Sr-CN catalyst and (c, d) over the Pt/0.15Sr-CN catalyst

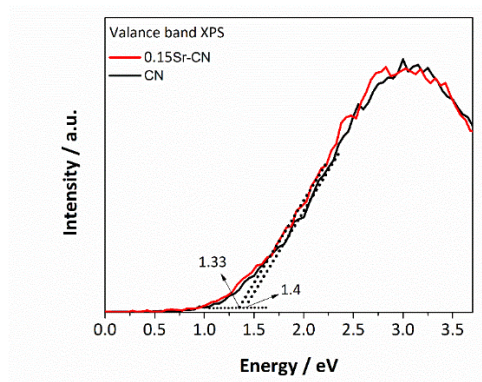




**Fig. S15** Visible light catalytic activities for H<sub>2</sub> evolution (a) of CN and xSr-CN samples (b) of CN, 0.15Sr-CN, Au/0.15Sr-CN and Pt/0.15Sr-CN samples. Photocatalytic recyclable tests for H<sub>2</sub> evolution (c) over the Au/0.15Sr-CN catalyst and (d) over the Pt/0.15Sr-CN catalyst



**Fig. S16** Visible light catalytic activities for RhB dye degradation (a) over CN and xSr-CN samples and (b) over CN, 0.15Sr-CN, Au/0.15Sr-CN and Pt/0.15Sr-CN samples. Visible light catalytic activities for 2,4-DCP degradation (c) over CN and xSr-CN samples and (d) over CN, 0.15Sr-CN, Au/0.15Sr-CN and Pt/0.15Sr-CN samples



**Fig. S17** Valence band XPS spectra of CN and 0.15Sr-CN samples

**Table S1** Total free energies of pristine CN and Sr-doped CN species

<i>Species</i>	<i>Total free energies</i>
Pristine CN	-15602.50103
Sr-CN (Interstitial)	-16534.02436
Sr-CN (C-substituted)	-16371.92395
Sr-CN (N-substituted)	-16251.95281

**Table S2** Work function, VBM, CBM, and band gap values in eV

<i>Species</i>	<i>Work functions</i>	<i>CBM</i>	<i>VBM</i>	<i>Bandgaps</i>
CN	5.84	-1.37	1.33	2.70
Sr-CN (Interstitial)	4.51	-2.74	-0.19	2.55
Sr-CN (C- substituted)	5.51	-1.08	1.05	2.13
Sr-CN (N- substituted)	4.73	-2.87	0	2.87

## S2 Quantum Efficiency Calculations for CO<sub>2</sub> Conversion

The quantum efficiency of CN, 0.15Sr-CN, Au/0.15Sr-CN and Pt/0.15Sr-CN samples for CO<sub>2</sub> conversion was calculated at  $\lambda=420$  nm. The samples were irradiated with a 300 W Xe-lamp for 8 h. The average incident irradiation was determined to be 2.01 mW cm<sup>-2</sup> by the Newport (Oriel instrument USA model 91150V ser. No 391/0118) and area of the light collector part was 6.5 cm<sup>2</sup>. The amount of CH<sub>4</sub> produced over the CN,

0.15Sr-CN, Au/0.15Sr-CN and Pt/0.15Sr-CN samples at  $\lambda=420$  nm was 1.4, 2.6, 4.35, and 4.8  $\mu\text{mol}$ , respectively. While, the amount of CO produced over the over the CN, 0.15Sr-CN, Au/0.15Sr-CN and Pt/0.15Sr-CN samples under same wavelength was 1.78, 3.85, 5.65 and 6.5  $\mu\text{mol}$ , respectively. The calculations are given below.

Quantum efficiency calculation for CN, 0.15Sr-CN, Au/0.15Sr-CN and Pt/0.15Sr-CN photocatalysts at  $\lambda=420$  nm: Number of incident photons (N) in 8 h over 6.5  $\text{cm}^2$  area:

$$N = \frac{E\lambda}{hc} = \frac{2.01 \times 10^{-3} \times 6.5 \times 420 \times 10^{-9} \times 8 \times 3600}{6.626 \times 10^{-34} \times 3 \times 10^8} = 7.9 \times 10^{20}$$

$$QE = \frac{\{(2 \times \mu\text{mol of CO}) + (8 \times \mu\text{mol of CH}_4)\} \times \text{Avogadro number}}{\text{the number of incident photons}} \times 100$$

$$QE_{\text{CN}} = \frac{\{(2 \times 1.78 \times 10^{-6}) + (8 \times 1.4 \times 10^{-6})\} \times 6.02 \times 10^{23}}{7.9 \times 10^{20}} \times 100 = 0.85\%$$

$$QE_{0.15\text{Sr-CN}} = \frac{\{(2 \times 3.85 \times 10^{-6}) + (8 \times 2.6 \times 10^{-6})\} \times 6.02 \times 10^{23}}{7.9 \times 10^{20}} \times 100 = 1.58\%$$

$$QE_{\text{Au}/0.15\text{Sr-CN}} = \frac{\{(2 \times 5.65 \times 10^{-6}) + (8 \times 4.35 \times 10^{-6})\} \times 6.02 \times 10^{23}}{7.9 \times 10^{20}} \times 100 = 2.65\%$$

$$QE_{\text{Pt}/0.15\text{Sr-CN}} = \frac{\{(2 \times 6.5 \times 10^{-6}) + (8 \times 4.8 \times 10^{-6})\} \times 6.02 \times 10^{23}}{7.9 \times 10^{20}} \times 100 = 2.92\%$$

**Table S3** Comparison of our results for CO<sub>2</sub> conversion with the previous reports

S.#	Photocatalysts	Source of light	Wavelength used	Quantum efficiency (%)	Refs.
1	NiS <sub>2</sub> QDs-g-C <sub>3</sub> N <sub>4</sub>	300 Xe-lamp	420 nm	2.03%	Colloid. & Surf. A: Phys. & Eng. Asp. 600, 2020, 124912.
2	CdSe/P-CN	300 Xe-lamp	420 nm	2.57%	Appl. Catal., B: Environ. 270, 2020, 118867
3	SnO <sub>2</sub> /B, P-gC <sub>3</sub> N <sub>4</sub>	300 Xe-lamp	420 nm	2.02%	Appl. Catal., B: Environ. 201, 2017, 486-494.
4	Pt/0.15Sr-CN	300 Xe-lamp	420 nm	2.92%	Current work