Carbon-vacancy modified graphitic carbon nitride: enhanced CO₂ photocatalytic reduction performance and mechanism probing

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Figure S1. High resolution XPS O 1s spectra of GCN and GCN510 samples.



Figure S2-1. N_2 adsorption/desorption isotherms of GCN, GCN510 and GCN-BET samples.



Figure S2-2. The pore-size distributions calculated from the desorption branch of GCN and GCN510 samples.



Figure S3. CO evolution on GCN and GCN510 photocatalysts in 4 h light ($\lambda \ge 420$ nm) illumination.



Figure S4. Schematic illustration of an example of nanometer-scale holes formation in GCN510.



Figure S5. Optimized geometry structure for CO₂ adsorption on (a) GCN surface and (b) carbon-vacancy modified GCN surface, where the green, gray, yellow and red color spheres represent C, N, H and O atoms, respectively.



Figure S6. (a) The XRD pattern, (b) UV-Vis diffuse reflectance spectra of GCN-BET compared with GCN and GCN510 samples, (c) and (d) TEM images of GCN-BET



Figure S7. (a) XPS survey spectra; high resolution XPS (b) O 1s, (c) C 1s, (d) N 1s spectra of GCN-BET sample.

From the above structure characterization, we can see that GCN-BET keeps a similar basic structure with the pristine GCN sample. And from the XPS analysis we can learn that the fitted peaks in C 1s spectra do not show an obvious shift toward high binding energy. At the same time, the area fraction of N-H/N-H₂ in N 1s spectra of GCN-BET is a little bit higher than GCN.