Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Selective hydrogen-deuterium exchange in graphitic carbon nitrides: probing the active sites for photocatalytic water splitting by solid-state NMR

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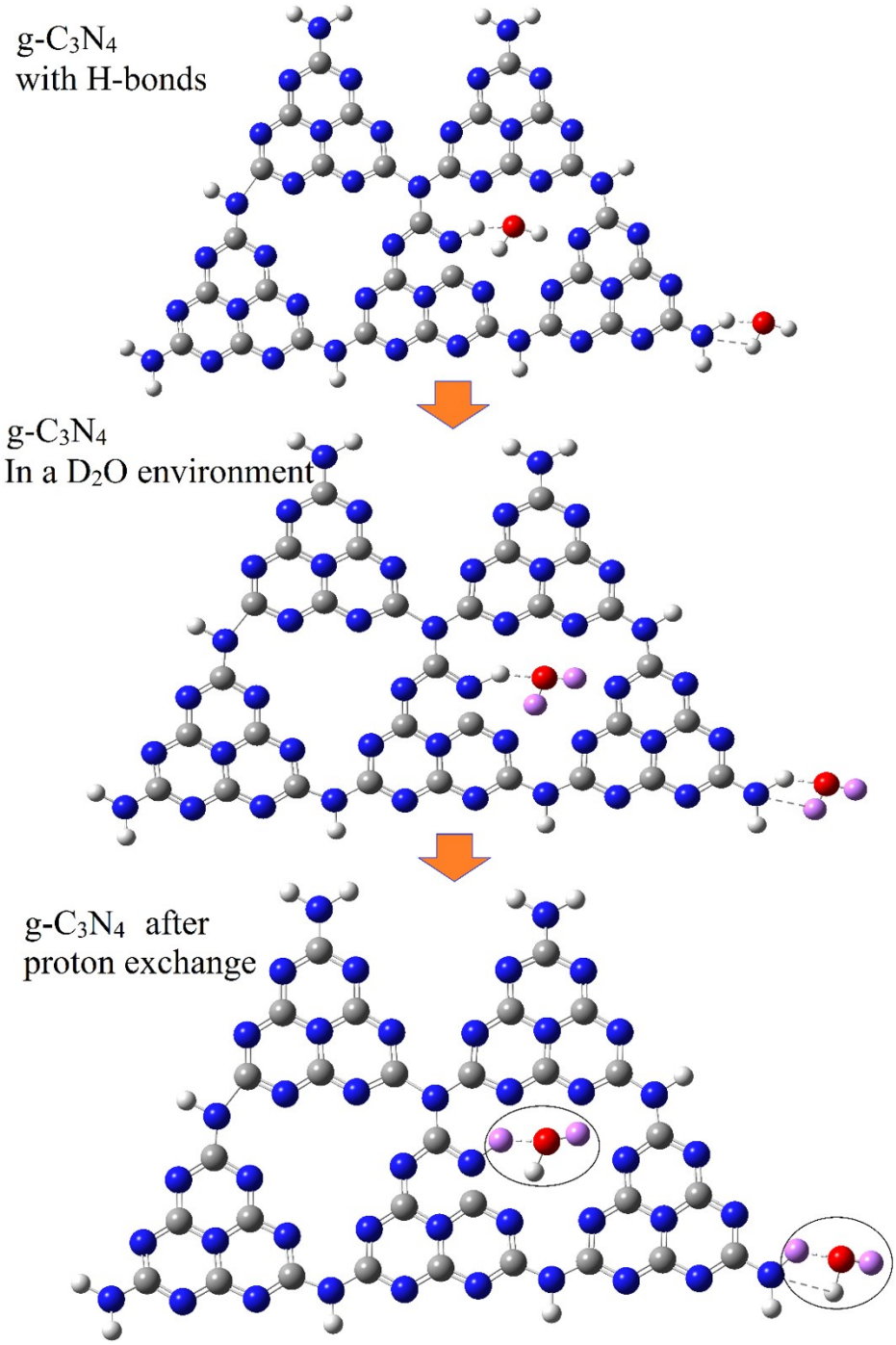

Figure S1. Schematic illustrating an idealized proton exchange process, where the nitrogen, carbon, hydrogen, oxygen, and deuterium atoms are given as blue, grey, white, red, and light purple spheres, respectively.

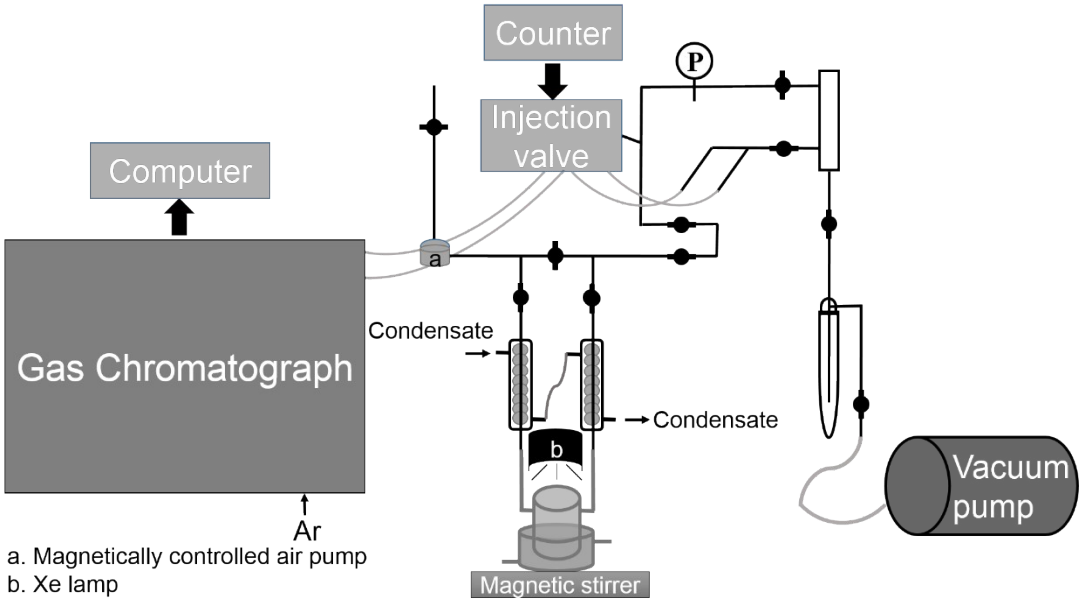

Figure S2. Photocatalysis instrument.

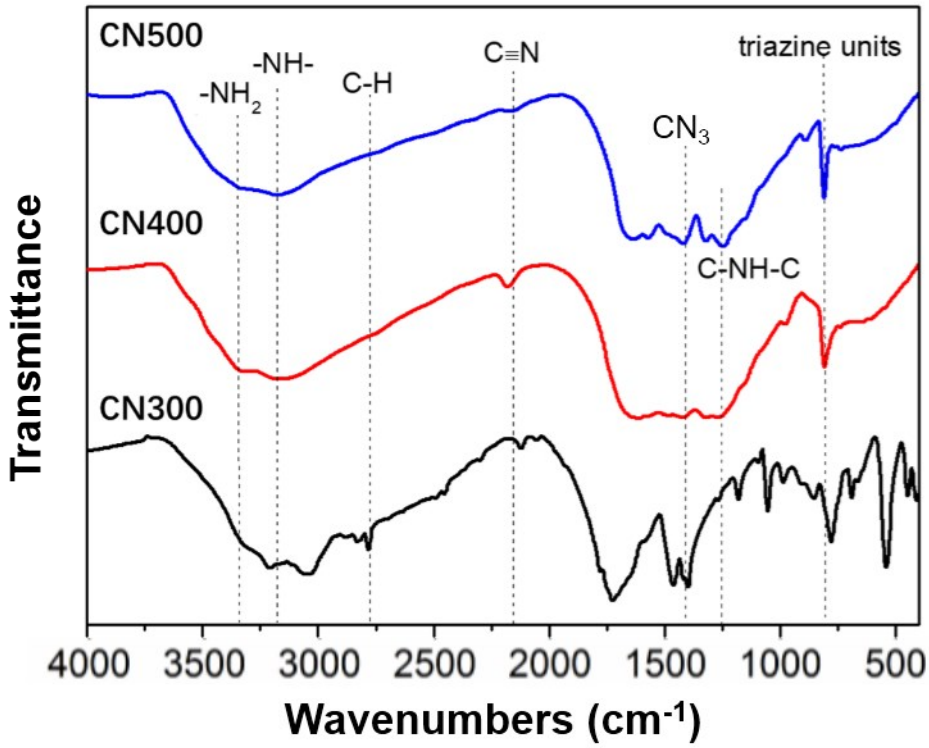

Figure S3. FTIR results for CN300, CN400, and CN500 samples.

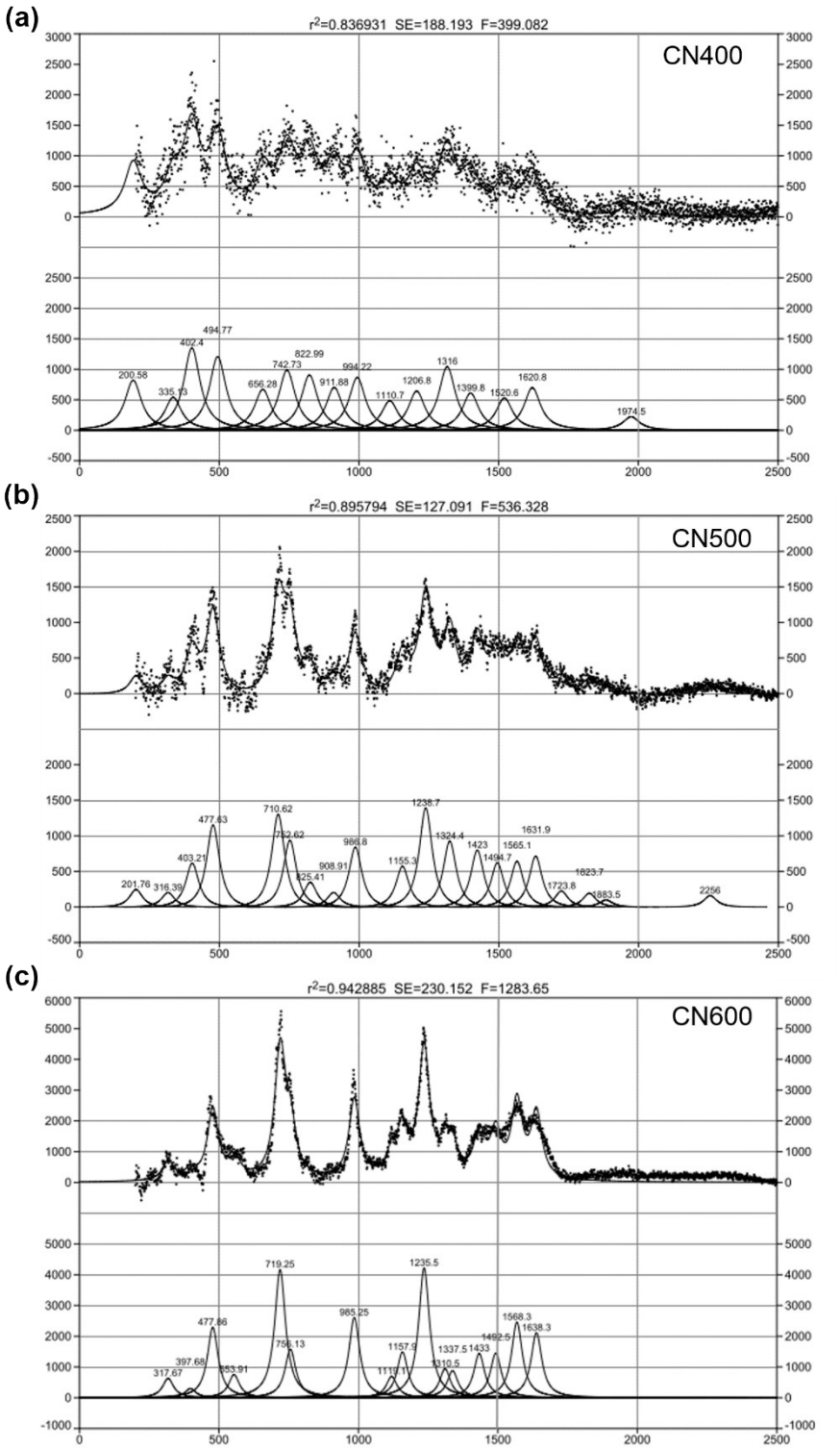

Figure S4. Raman spectra of CN400, CN500, and CN600 samples.

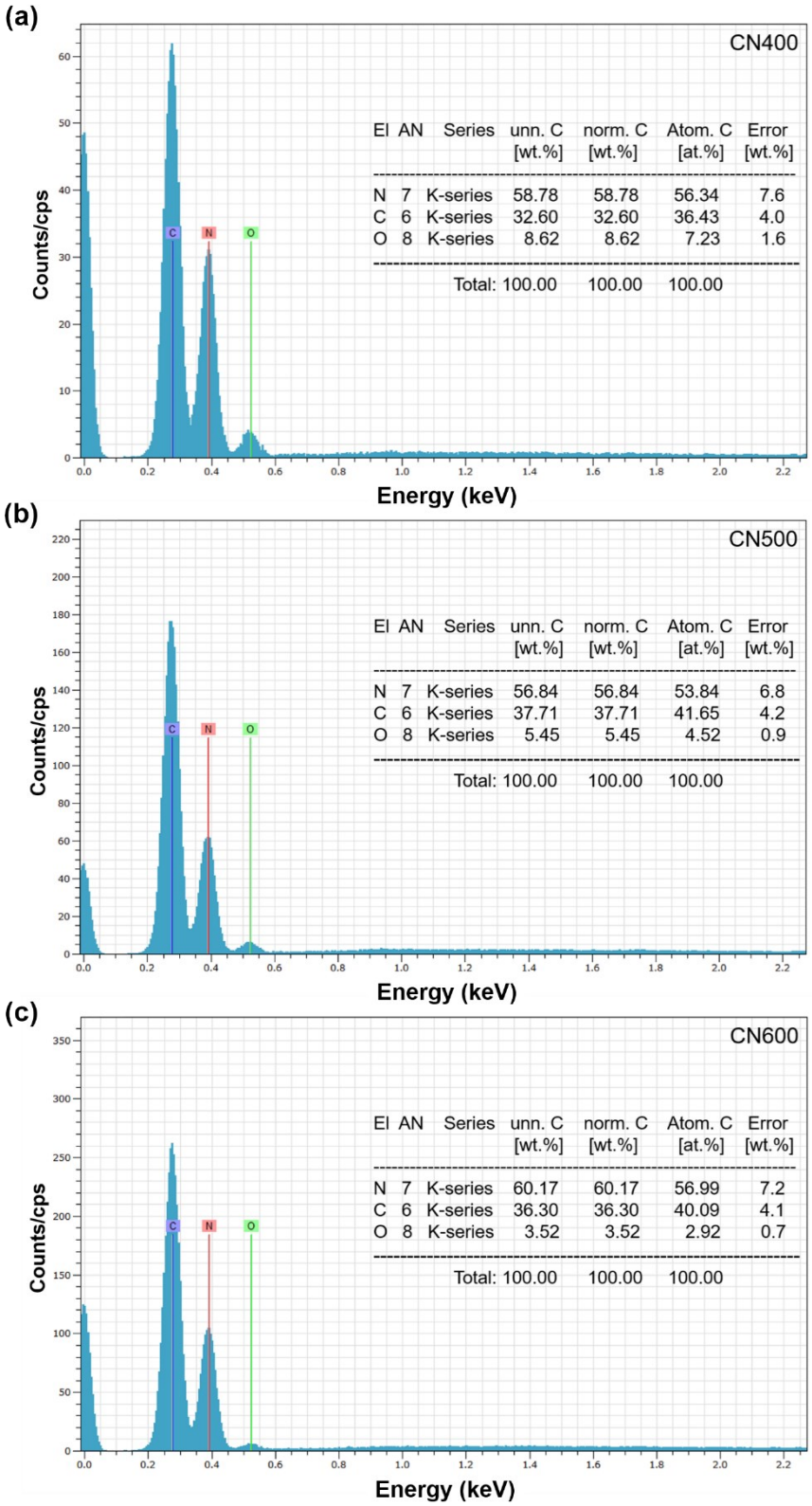

Figure S5. EDS analyses of CN400, CN500, and CN600 samples.

The proportions of C, N, and O in the as-synthesized CN400, CN500, and CN600 samples were also examined by energy dispersive X-ray spectroscopy (EDS), and the results are presented as Supplemental information (Figure S4) to conserve space. The atomic C:N ratios calculated from the C and N peaks of the EDS spectra for the CN400, CN500, and CN600 samples were about 0.65, 0.78, and 0.70, respectively, which is approximately consistent with the values presented in Table 1. As discussed, deviations from the theoretical C:N ratio of 0.75 can be attributed to defects in the prepared sample structure due to residual $–NH_2$-, NH-, or –CH- groups. We also note that the proportion of O in CN400 (7.23 at%) is relatively high, but this decreases with increasing calcination temperature to 4.52 at% for CN500 and 2.92 at% for CN600, as was observed in Table 1.

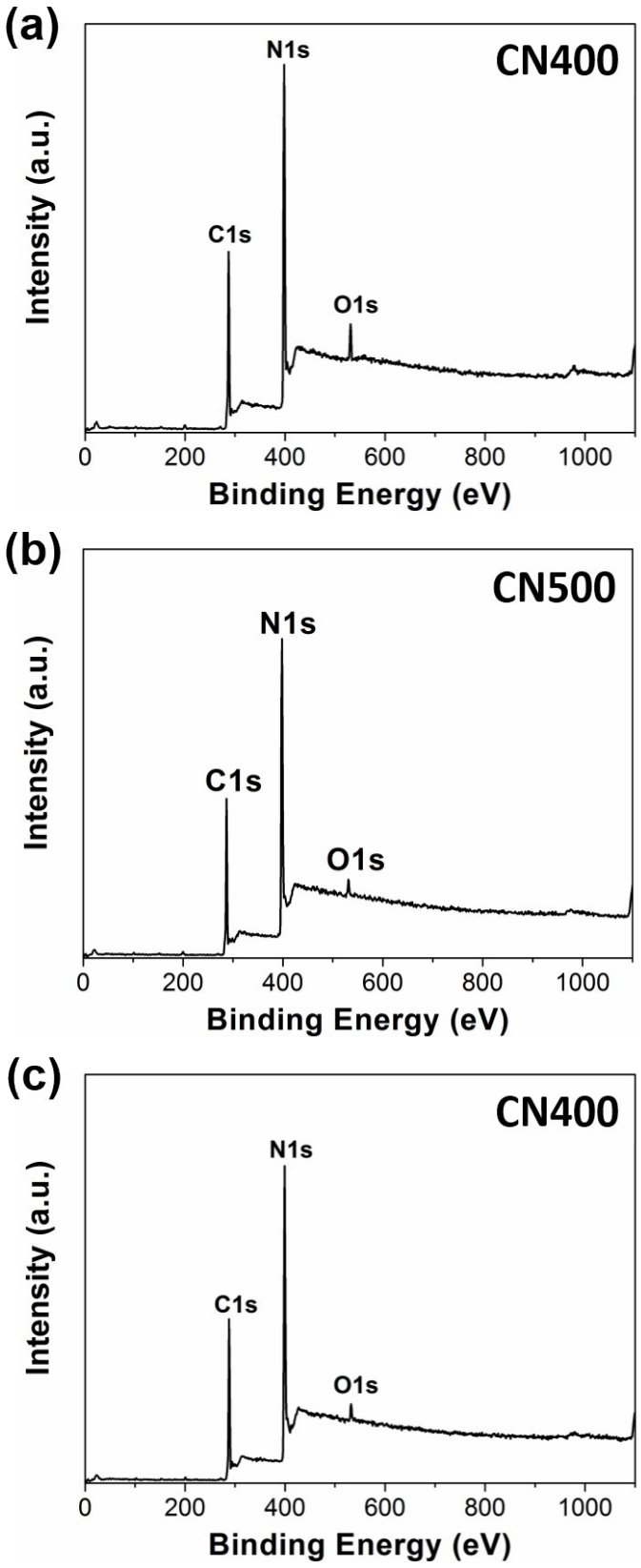

Figure S6. Full-scan XPS spectra for (a)CN400, (b)CN500, and (c)CN600.

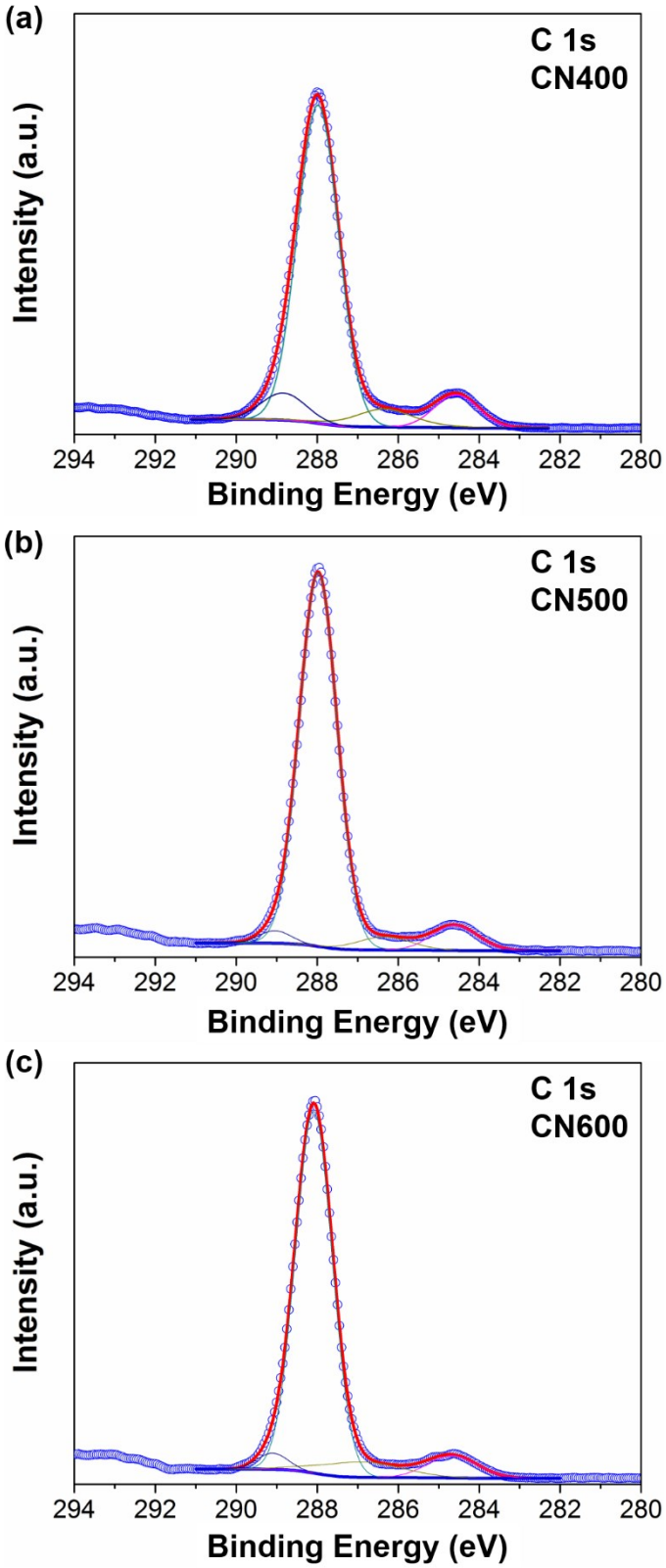

Figure S7. C 1s XPS spectra of (a)CN400, (b)CN500, and (c)CN600.

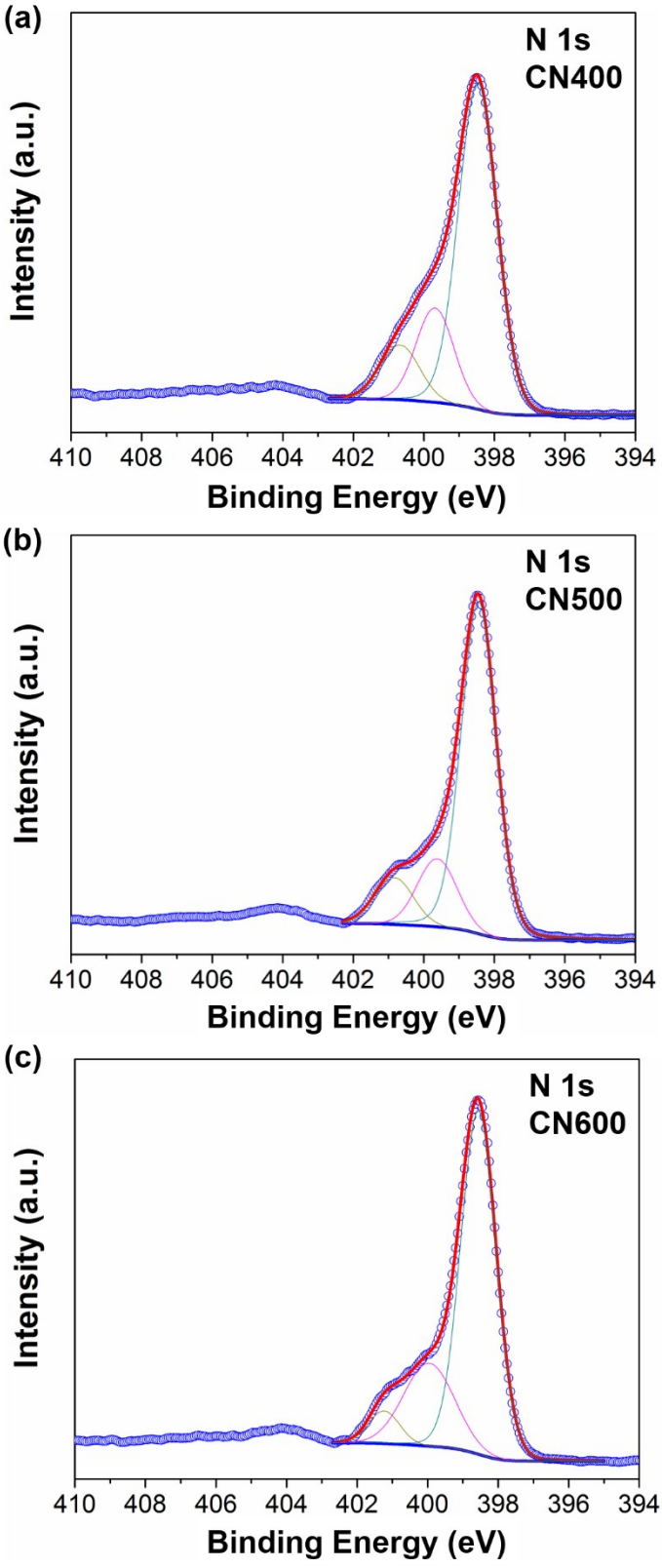

Figure S8. N 1s XPS spectra of (a)CN400, (b)CN500, and (c)CN600.

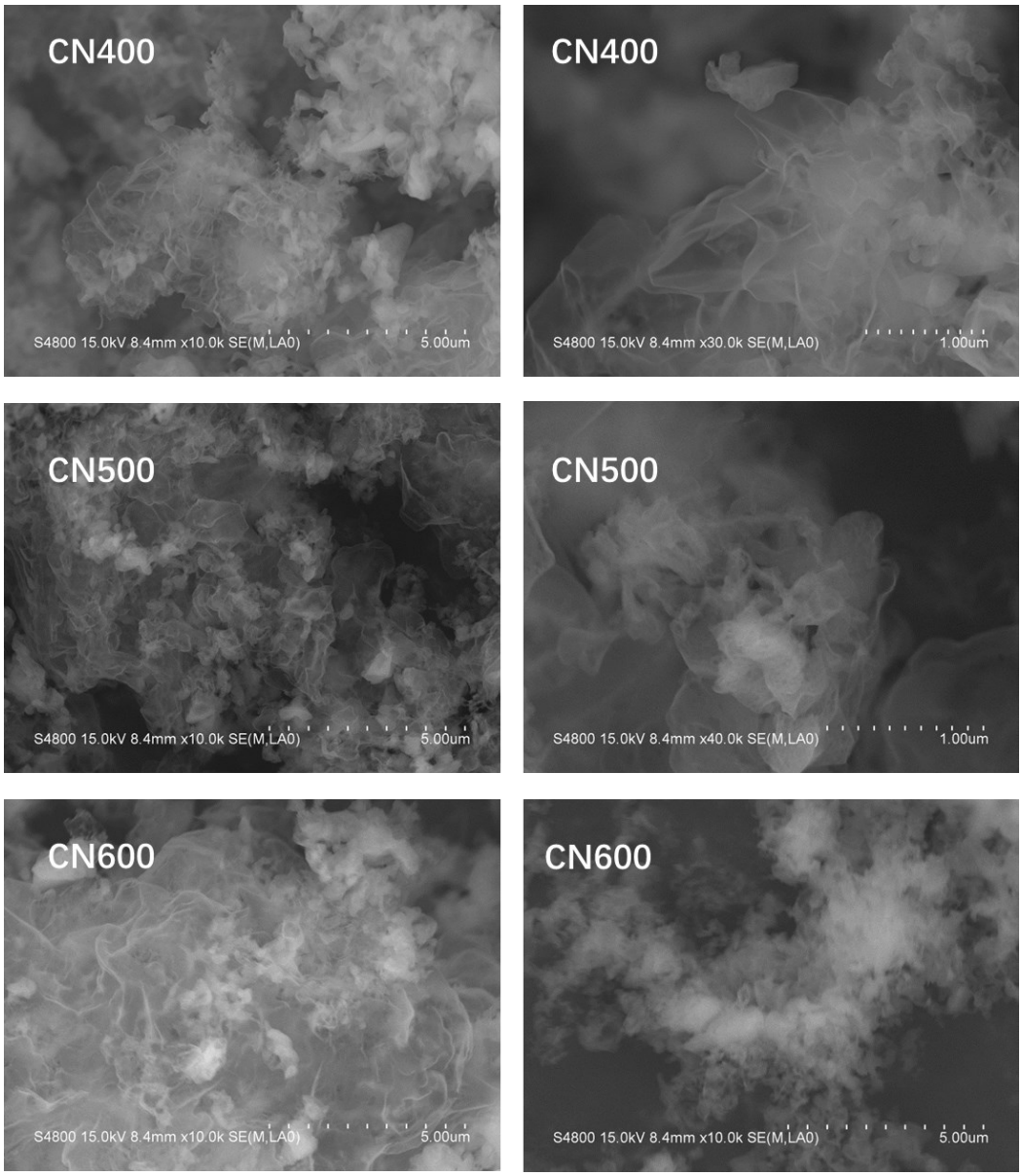

Figure S9. SEM images of CN400, CN500, and CN600.

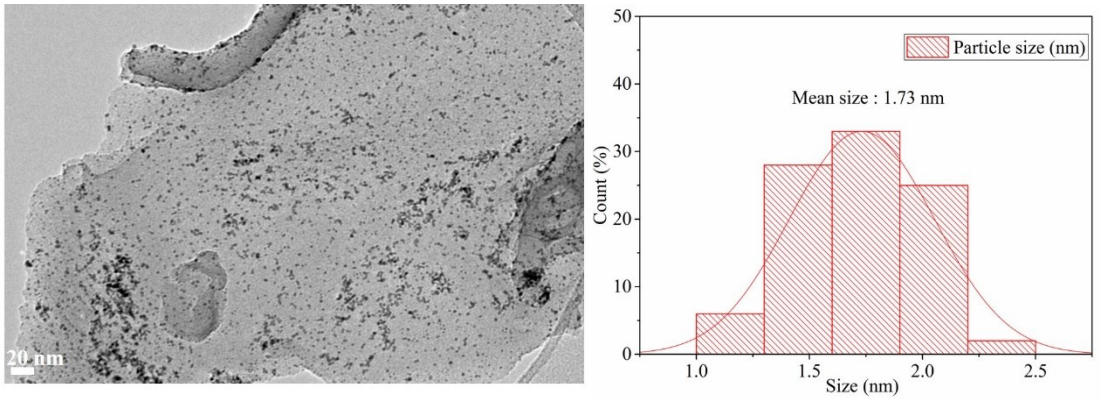

Figure S10. TEM image and the distribution of particle size for CN500 samples.

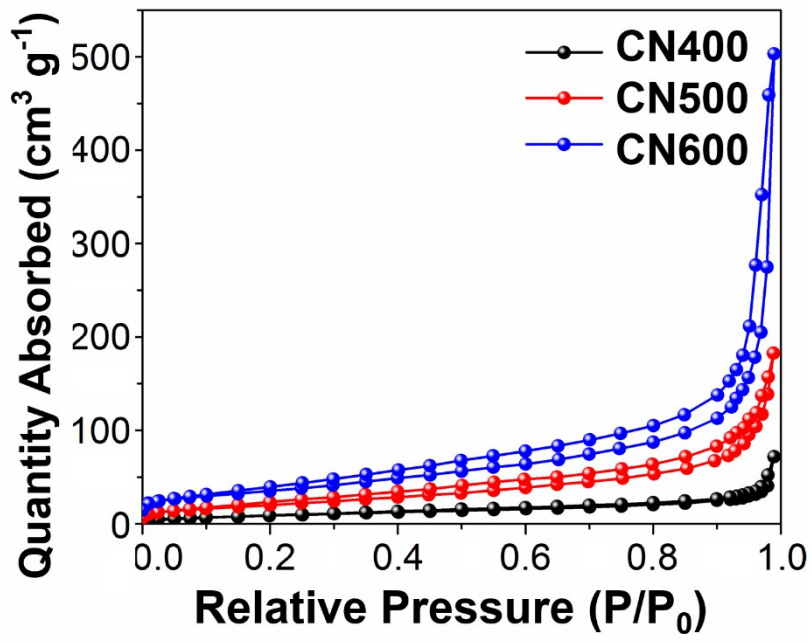

Figure S11. Nitrogen adsorption-desorption isotherms of CN400, CN500, and CN600.

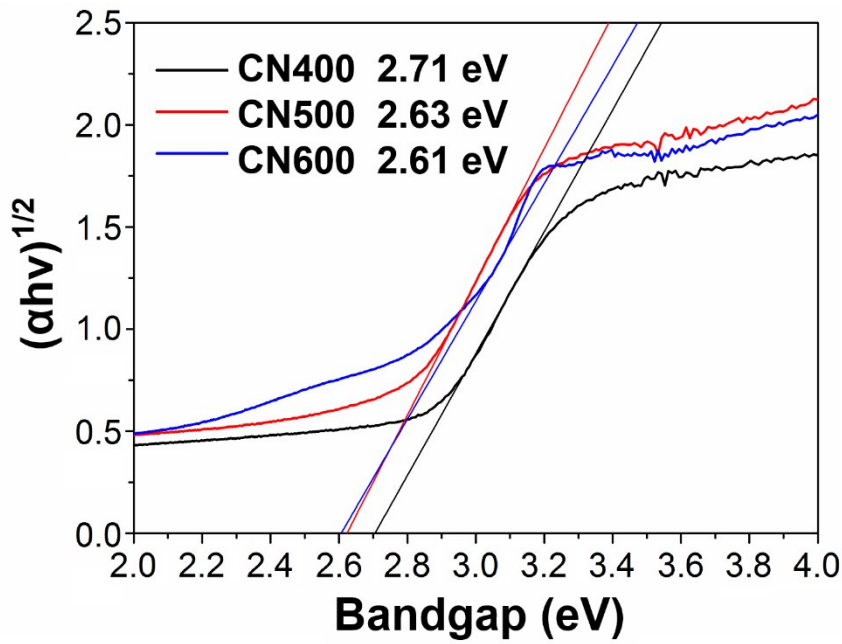

Figure S12. Tauc plots of CN400, CN500, and CN600 samples, which plot the value $(\alpha h\nu)^{1/2}$, where α is the optical absorption coefficient of the material, versus the photon energy hv obtained from ultraviolet-visible diffuse reflection spectroscopy (UV-Vis DRS) results.

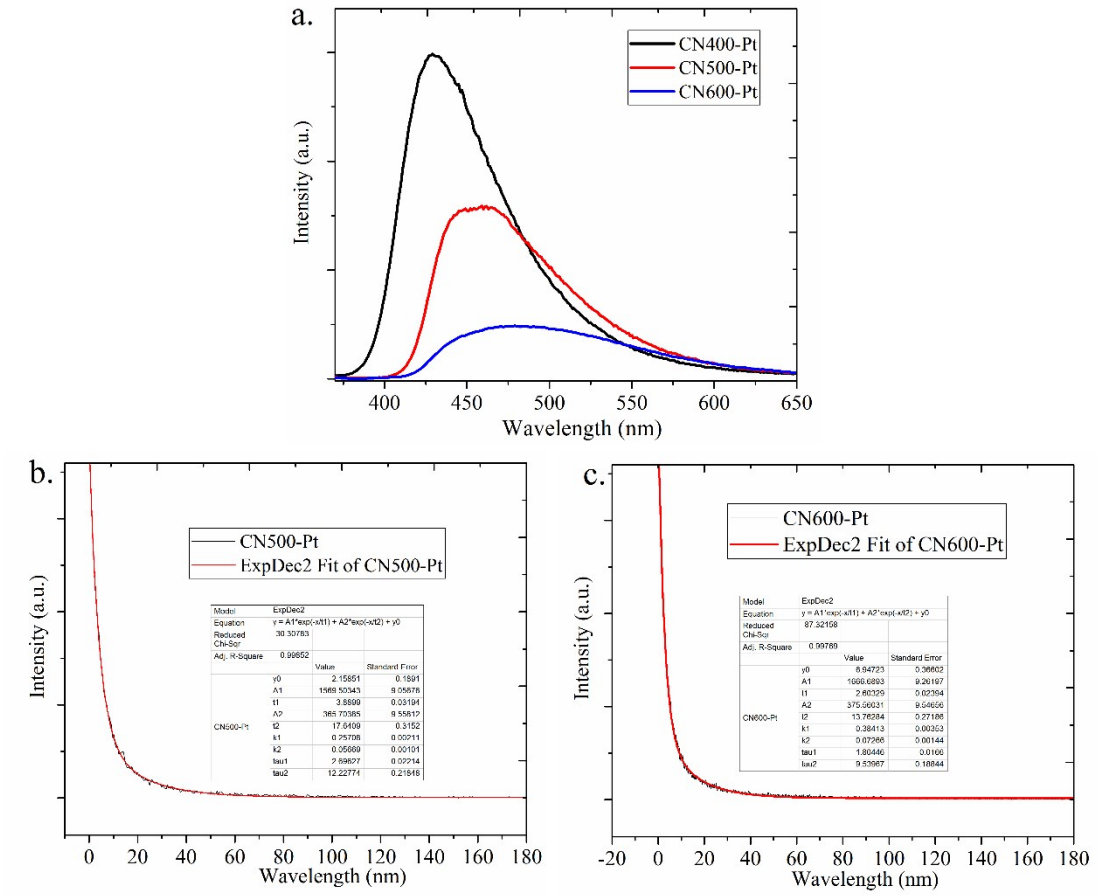

Figure S13. (a) Photoluminescence spectra for CN300-Pt, CN400-Pt and CN500-Pt. Time resolved emission spectroscopy for (b) CN500-Pt and (c) CN600-Pt.