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Supplemental Information for

Giant nonlinear optical responses of carbyne

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Figure S1. The spectrum characterization of carbyne. (a) UV-Vis spectrum. (b) XRD pattern. The XRD pattern shows clean, shape, strong peaks, indicating carbyne crystals with good crystallinity. These peaks are indexed to the hexagonal structure of carbyne. Note that there is an obvious preferred orientation along the c-axis. (c)The micro-Raman spectra (514 nm laser source) of the samples show two sharp peaks, at 1050 and 2175 cm^{-1}, which are identified as the characteristic peaks of carbon–carbon single bonds and triple bonds, respectively, of carbyne. (d) FTIR spectrum. The signal in the FTIR spectrum at 2168 cm^{-1} is in agreement with the reported value for carbon–carbon triple bonds, between 2000 and 2200 cm^{-1}.

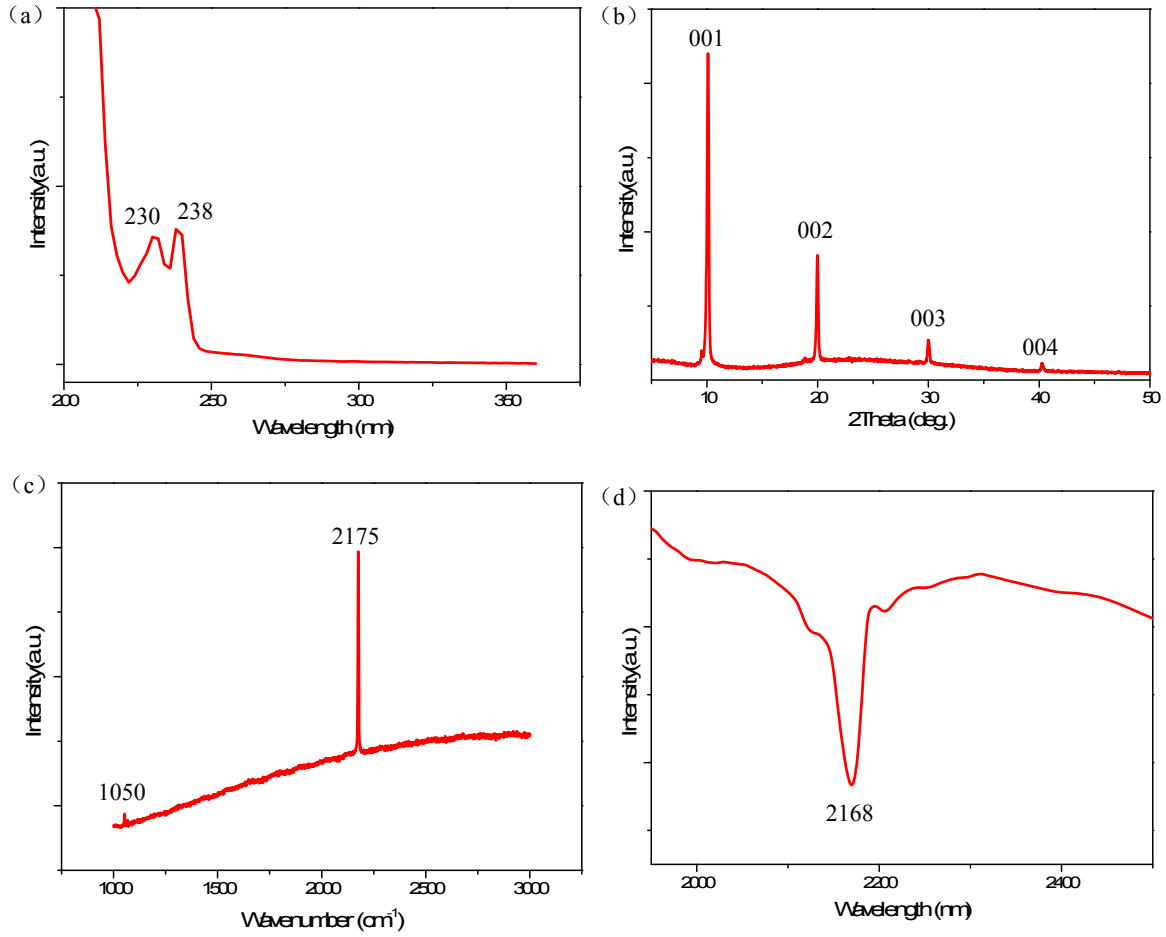

Figure S2. The FTIR spectrum of carbyne (Black line). The signal located at near 1500 and 2850-3000 cm^{-1} represent the CH_2 or CH_3 bending and stretching vibration. The peak at 1750 cm^{-1} belongs to the signal of C=O and the peak near 2160 cm^{-1} comes from the stretching vibration of C≡C bond. The FTIR spectrum of alcohol is taken for comparison (Red line).

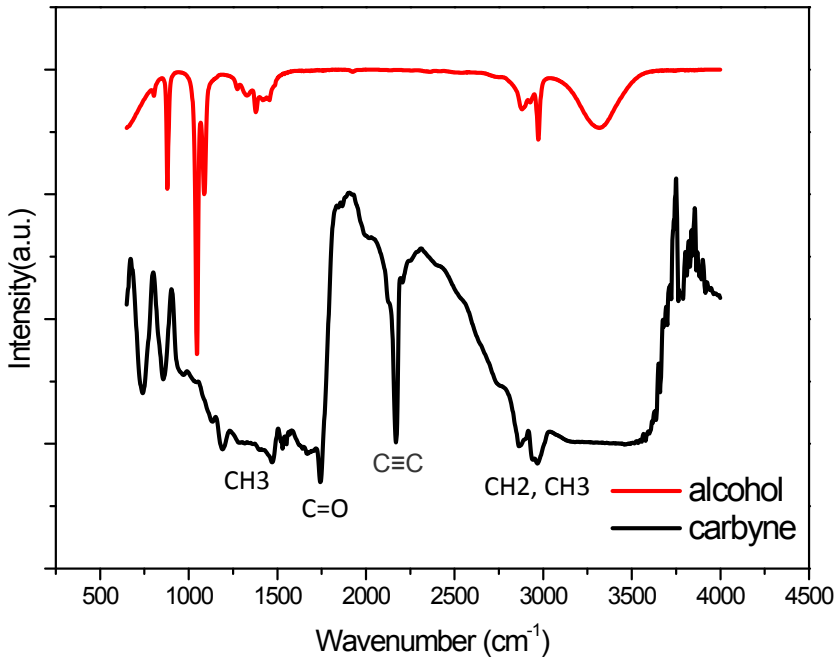

Figure S3. SEM and TEM images.(a) SEM image of carbyne crystals. They are in the shape of flakes, which are stacking together. (b) TEM image of carbyne crystals with rod-like morphology. (c-d) SAED patterns and HRTEM images are based on the [001]directions of incident electron beam.