Supplementary information

g-C$_3$N$_4$ and Tetrabutylammonium bromide catalyzed efficient conversion of Epoxide to Cyclic Carbonate under ambient condition

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Experimental Section:

Materials.

Melamine was purchased from LOBA Chemicals. tetrabutylammonium bromide (TBAB) was purchased from SRL. All epoxides used here were purchased from sigma aldrich. Chloroform-d was purchased from sigma and chloroform was used as internal standard. All chemicals were used as received.

Experimental Procedure.

Prepared g-C$_3$N$_4$ was characterized by PXRD, FTIR, solid state $^{13}$C NMR (CP MAS) and, TGA analysis. Cyclic carbonates produced by the reaction of epoxide and CO$_2$ was characterized by solution state $^1$H and $^{13}$C NMR spectroscopy.

General Procedure: 13.7 mmol epoxides, g-C$_3$N$_4$ and TBAB were taken in 50 ml Schlenck round bottom flak with a small magnetic stirrer. One blank glass tube was kept as condenser above the round bottom flask. On the top of the glass tube, the balloon attached with the glass stopcock was fitted. All glass joints were sealed with both grease and teflon tape in order to minimize the gas lick-age. Subsequently, the set up was vacuumed and backfill with 99.995% CO$_2$ gas thrice to remove any dissolved air from the setup and heating was started. Subsequently, the reaction mixture was heated for 20 hours in the CO$_2$ environment. After the completion of the reaction, a small amount of the reaction mixture was taken in CDCl$_3$ and immediately precipitate of g-C$_3$N$_4$ appeared. Precipitates were separated by centrifugation and the solution was utilized for NMR measurement.

Recyclability Test:

Recyclability was checked using epichlorohydrin as substrate. For every cycle 13.7 mmol epoxides was added to the reaction mixture and using the CO$_2$ balloon reaction was started. In order to check the conversion small amount of aliquot was taken for $^1$H NMR analysis. The results showed complete conversion.
Fig. S1: Experimental setup for g-C$_3$N$_4$ & TBAB catalyzed epoxide to cyclic carbonate conversion.

Fig. S2: PXRD spectrum of g-C$_3$N$_4$. 

Intensity (a.u.)

2θ (degree)
Fig. S3. Thermogravimetric analysis curves of g-C3N4.
Fig. S4: $^{13}$C (CP MAS) NMR of g-C$_3$N$_4$ (500 MHz).

Fig. S5: IR Spectra of melamine and g-C$_3$N$_4$. 

Transmittance (a.u.)

N-H
3645-3020

C-N
1645-1225

Wave number (cm$^{-1}$)
Fig. S6: 4-(chloromethyl)-1,3-dioxolan-2-one: $^1$H NMR (CDCl$_3$, 500 MHz).

Fig. S7: 4-phenyl-1,3-dioxolan-2-one: $^1$H NMR (CDCl$_3$, 400 MHz).
Fig. S8: 4-(phenoxyethyl)-1,3-dioxolan-2-one: $^1$H NMR (CDCl$_3$, 400 MHz).
Fig. S9: 4-(allyloxymethyl)-1,3-dioxolan-2-one: $^1$H NMR (CDCl$_3$, 500 MHz).
Fig. S10: 4-(oct-7-enyl)-1,3-dioxolan-2-one: 1H NMR (CDCl₃, 400 MHz).
Fig. S11: hexyl-1,3-dioxolan-2-one: $^1$H NMR (CDCl$_3$, 400 MHz).
Fig. S12: 4-butyl-1,3-dioxolan-2-one: $^1$H NMR (CDCl$_3$, 400 MHz).
Fig. S13: Schematic illustration of the different pathways for CO$_2$ absorption by g-C$_3$N$_4$. 