Efficient synthesis of epoxybutane from butanediol via a twostep process

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Figure S1 The device for the continous decarboxylation process.



Figure S2 (a) CO_2 –TPD, (b) NH_3 –TPD of the $NaAlO_2$



Figure S3 XRD patterns obtained for $NaAlO_2$: (a) fresh $NaAlO_2$, (b) used $NaAlO_2$.



Figure S4 FTIR spectra obtained for $NaAlO_{2:}$ (a) Fresh $NaAlO_{2}$, (b) recovered $NaAlO_{2}$.



Figure S5 CO_2 -TPD of the NaAlO₂ (both before and after reaction)

Table S1 The BET of the $NaAlO_2$ (both before and after reaction)

Catalyst	BET surface area (m 2 g $^{-1}$)
fresh NaAlO ₂	1.7
used NaAlO ₂	13.6



Figure S6. Effect of the catalyst type on the FR_{BO} of the decarboxylation of butenyl carbonate. (Reaction conditions: BC: 40g; catalyst:2g; temperature: 185 °C; reaction time: 2h; vacuum degree: 0.005 MPa.)







TS1



A





TS2

TS3







Figure S7 Reaction pathways to produce BO



reaction.

The structure of BO produced from the consecutive carbonylation and decarboxylation was also determined by ¹H-NMR analysis. As illustrated in Figure S2. There are five characteristic peaks corresponding to different protons in these spectra. The signals at 1.02 ppm was attributed to the methyl protons of BO (CH₃); δ 1.58 ppm was ascribed to the methylene protons of BO (CH₂); δ 2.74 ppm is attributed to the methyne proton of BO (CH); the two singlets at 2.48 and 2.89 ppm are attributed to the protons of BO. The ¹H-NMR results further verified that there are no other impurities in BO. Above all, in this work, the decarboxylation of BC was successfully conducted and remarkable results were achieved over [Bmim][Br] catalyst.