

Supporting Information

## **Coupling hydrogen bond donors and atomically dispersed Zn-N<sub>4</sub> sites in porous n-doped carbon for CO<sub>2</sub> fixation to cyclic carbonates**

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### *NH<sub>3</sub>-TPD test*

NH<sub>3</sub>-TPD was carried out on a conventional apparatus with an online thermal conductivity detector. Generally, the sample (0.1 g) was heated to 200 °C in a flow of N<sub>2</sub> with high purity for 2 h, and then cooled down to the ambient temperature. After that, sufficient NH<sub>3</sub> was introduced into the system and the physically adsorbed NH<sub>3</sub> was then removed by flushing with N<sub>2</sub> at 100 °C for 2 h and the desorption process was performed by heating the sample from 50 to 300 °C at a rate of 10 °C/min.

### *The recyclability and versatile applicability of the catalysts*

When the reaction was over, ZNCs was recycled by centrifugation, washed with ethanol and dried at 80 °C for the next cycle of test. Besides epichlorohydrin, other kinds of epoxides such as epibromohydrin (98%, Aladdin Industrial, China), styrene oxide (99%, Aladdin Industrial, China), benzyl(R)-(-)-glycidyl ether (99.0%, Aladdin Industrial, China), 1,2-epoxyhexane (96%, Aladdin Industrial, China), cyclohexene oxide (98%, Aladdin Industrial, China), and glycidyl phenyl ether (99%, Energy Chemical, China) were also tried to estimate the substrate tolerance of catalysts.

### *Calculation of yield of target product*

The conversion and selectivity were calculated based on Eqs. (S1 and S2).<sup>1</sup>

$$\text{Conversion (\%)} = (C_0 - C_t) / C_0 \times 100\% \quad (\text{S1})$$

$$\text{Selectivity (\%)} = C_c / (C_0 - C_t) \times 100\% \quad (\text{S2})$$

where  $C_0$  and  $C_t$  represent the concentration of epoxide at 0 and  $t$  h and  $C_c$  represents the concentration of cyclic carbonate. The yield of target cyclic carbonate was calculated via multiplying selectivity by conversion. When the reaction was over, the catalyst was separated from the solution by centrifugation, washed by ethanol for several times and dried at 80 °C for the next cycle of test.

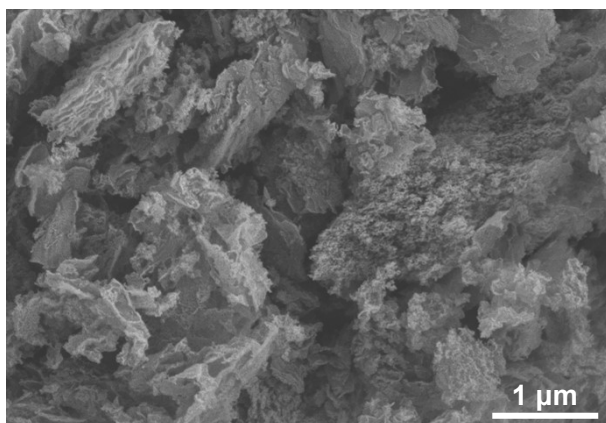


Fig. S1 SEM image of ZNC-800.

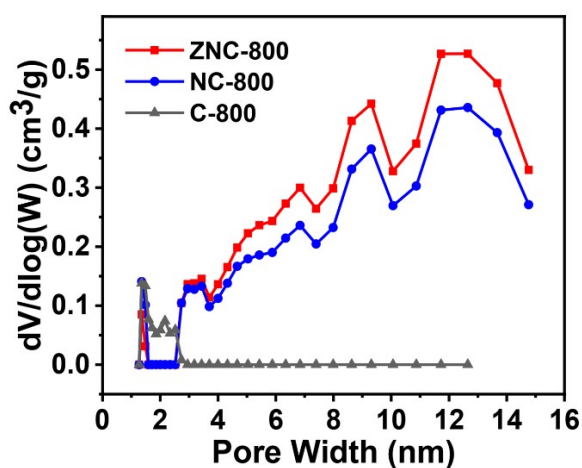


Fig. S2 Pore size distribution of C-800, NC-800 and ZNC-800.

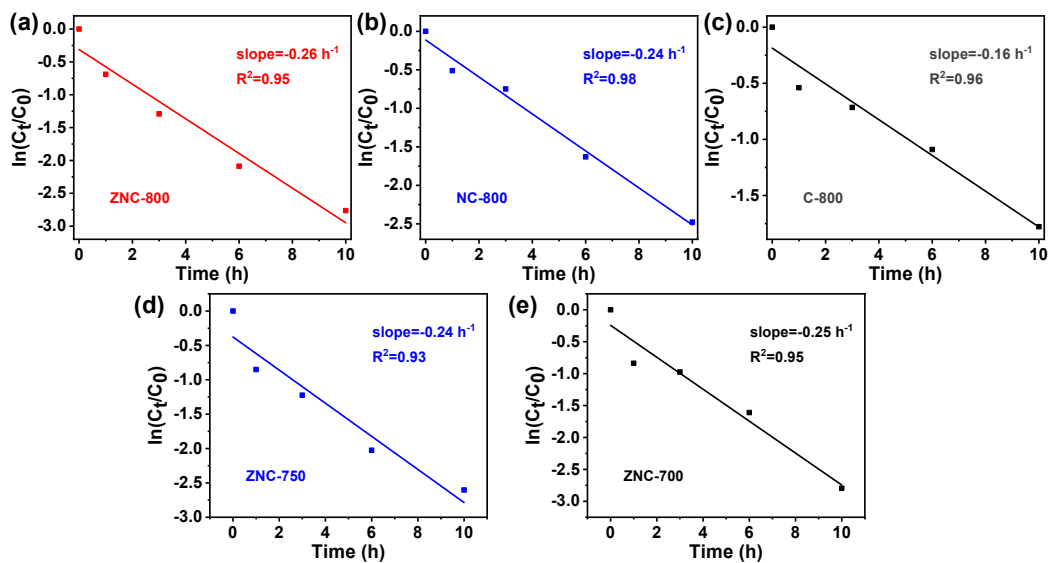


Fig. S3 Reaction kinetics curves of (a) ZNC-800, (b) NC-800, (c) C-800, (d) ZNC-750 and (e) ZNC-700.

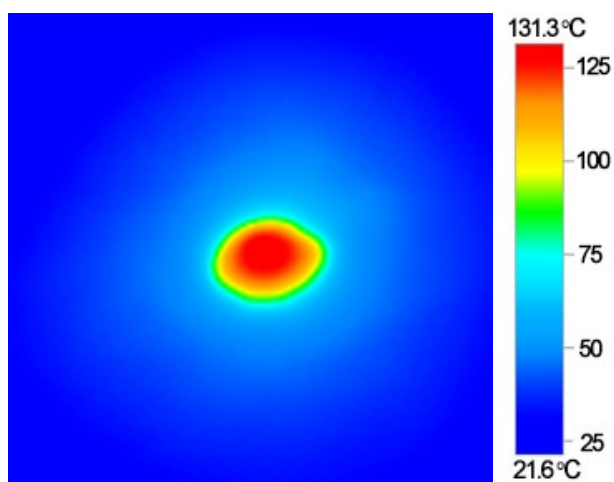
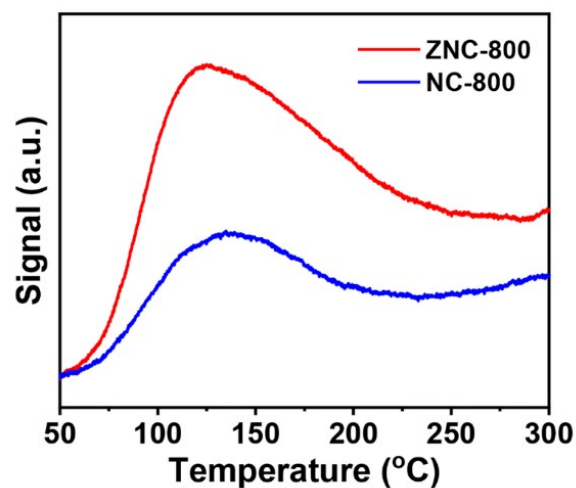


Fig. S4 Infrared radiation image of the ZNC-800 powder under light irradiation.



**Fig. S5** NH<sub>3</sub>-TPD of NC-800 and ZNC-800 (the peak area can roughly reveal the concentration of Lewis acidity, and clearly ZNC-800 has a larger peak area than NC-800, suggesting ZNC-800 has a higher concentration of Lewis acidity).

**Table S1** The content of each element in samples based on EDX analysis

	C (wt%)	O (wt%)	N (wt%)	Zn (wt%)
C-800	91	9	-	-
NC-800	70	9	21	-
ZNC-800	59	10	24	7

## References

1. M. Zhou, J. Chen, Z. Qu, Y. Du, J. Zhang, H. Jiang and R. Chen, *Sep. Purif. Technol.*, 2023, **320**, 124120.