catalysts

MDPI

Supporting Information

# Facile Synthesis of Silicon-Based Materials Modified using Zinc(II) 2-Bromoacetic as Heterogeneous Catalyst for the Fixation of $CO_2$ into Cyclic Carbonates

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## Catalyst characterization

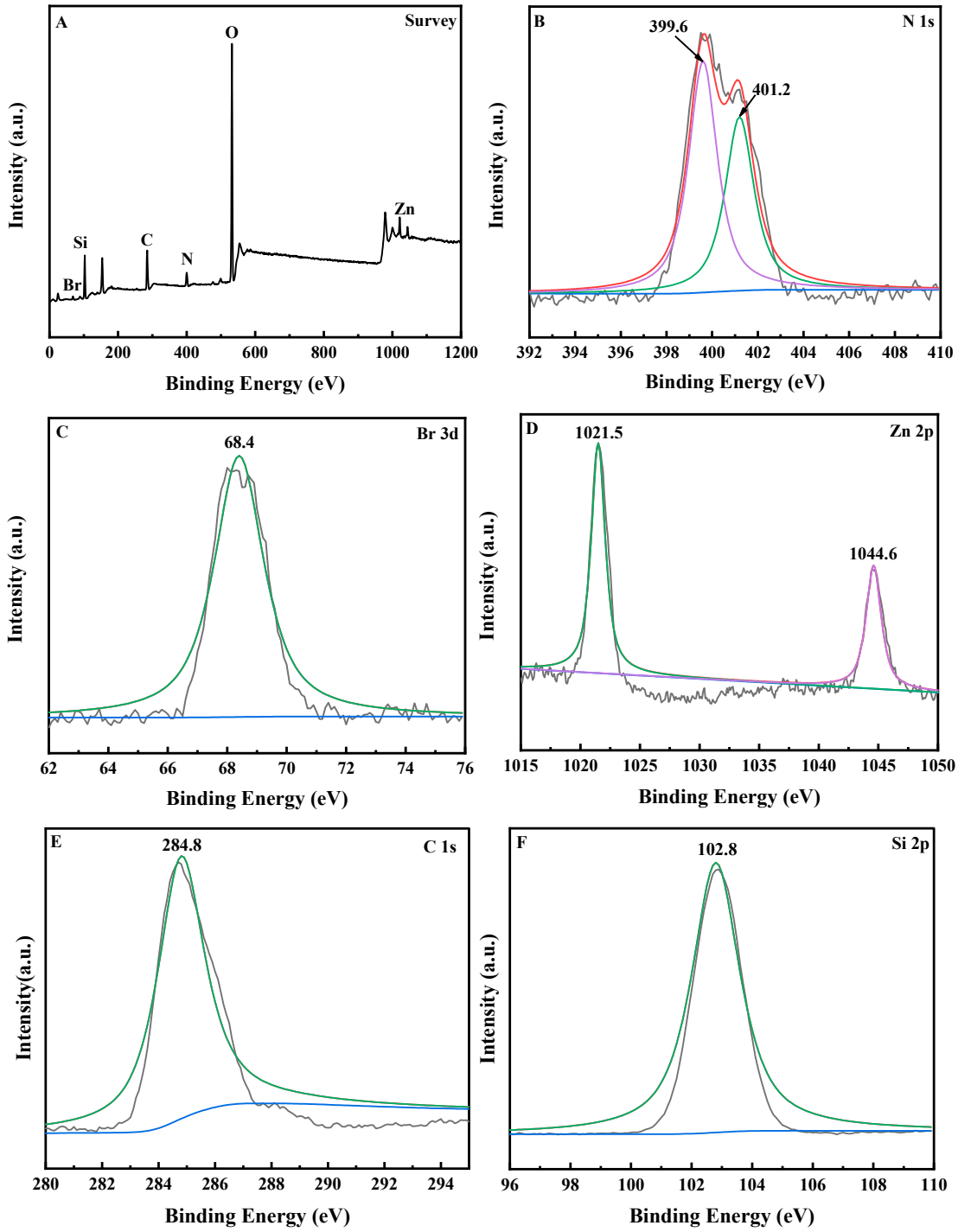


**Figure S1.** (**A**) Full spectrum; (**B**) N 1s XPS spectra; (**C**) Br 3d XPS spectra; (**D**) Zn 2p XPS spectra; (**E**) C 1s XPS spectra and (**F**) Si 2p XPS spectra of Si-ZnBA-2.

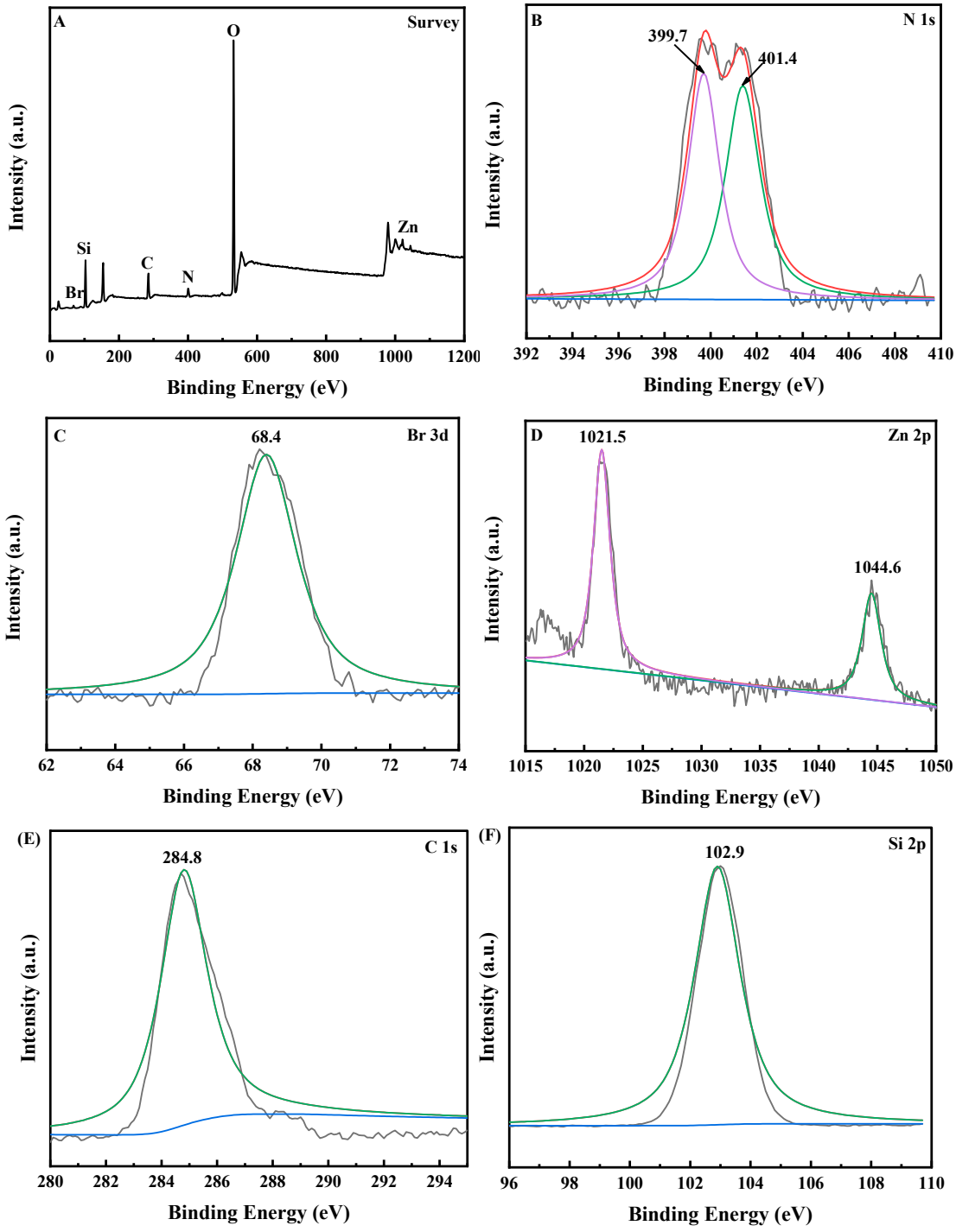


**Figure S2.** (**A**) Full spectrum; (**B**) N 1s XPS spectra; (**C**) Br 3d XPS spectra; (**D**) Zn 2p XPS spectra; (**E**) C 1s XPS spectra and (**F**) Si 2p XPS spectra of Si-ZnBA-3.

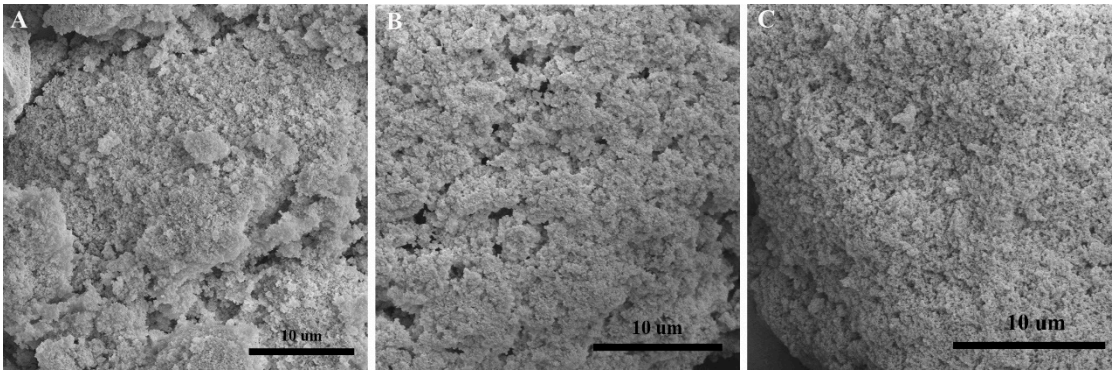


**Figure S3.** SEM images of (A) Si-ZnBA-1; (B) Si-ZnBA-2; (3) Si-ZnBA-3.

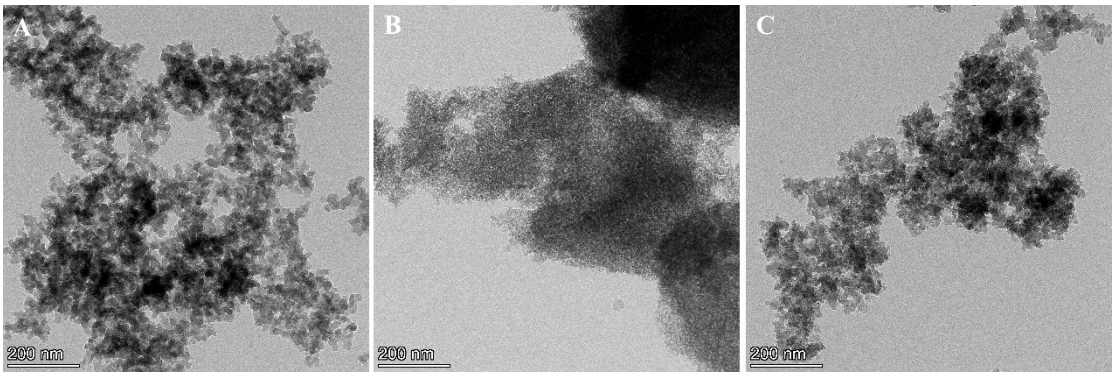


**Figure S4.** TEM images of (A) Si-ZnBA-1; (B) Si-ZnBA-2; (3) Si-ZnBA-3.

## Catalyst Performance Discussion

**Table S1.** Screening of catalyst [a].

| Entry | Catalyst | cocatalyst | Reaction results [b] | |
|---|---|---|---|---|
| | | | Yield /% | Selectivity /% |
| 1 | Si-ZnBA-2 | KI | 71 | ≥99 |
| 2 | Si-ZnBA-2 | KBr | 13 | ≥98 |
| 3 | Si-ZnBA-2 | KCl | trace | — |
| 4 | Si-ZnBA-2 | TBAI | 44 | ≥99 |
| 5 | Si-ZnBA-2 | TBAB | 24 | ≥99 |
| 6 | Si-ZnBA-3 | KI | 59 | ≥99 |
| 7 | Si-ZnBA-3 | KBr | 8 | ≥99 |
| 8 | Si-ZnBA-3 | KCl | trace | — |
| 9 | Si-ZnBA-3 | TBAI | 40 | ≥99 |
| 10 | Si-ZnBA-3 | TBAB | 24 | ≥99 |

[a] Reaction conditions: PO 34.5 mmol, 130 °C, 2.0 MPa, 5 h, Si-ZnBA-n 150 mg, co-catalyst 100 mg; [b] PC yield, PC selectivity all based on GC.

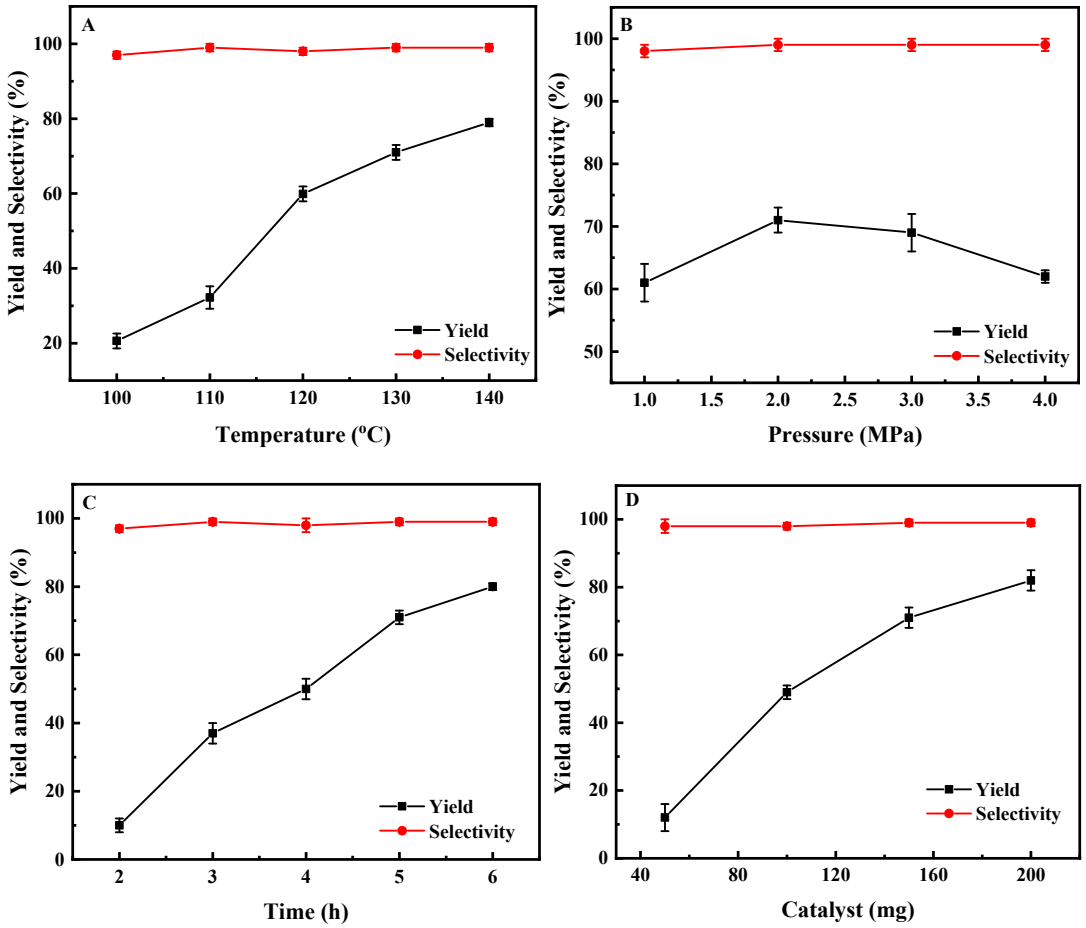


**Figure S5.** Effects of reaction conditions on PC synthesis. Reaction conditions: PO 34.5 mmol, KI 0.54 mmol, (**A**) Si-ZnBA-2 150 mg, 2.0 MPa, 5.0 h; (**B**) Si-ZnBA-2 150 mg, 130 °C, 5.0 h; (**C**) Si-ZnBA-2 150 mg, 130 °C, 2.0 MPa; (**D**) 130 °C, 2.0 MPa, 5.0 h.

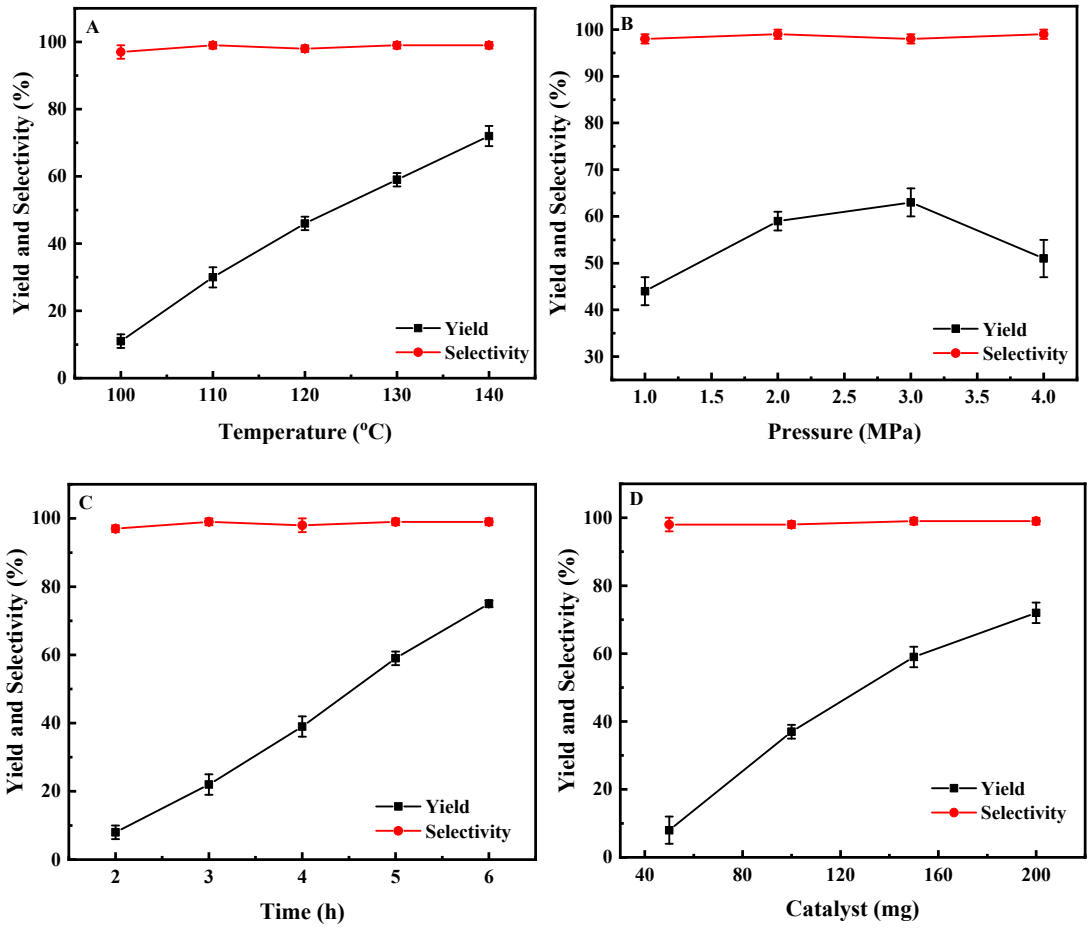


**Figure S6.** Effects of reaction conditions on PC synthesis. Reaction conditions: PO 34.5 mmol, KI 0.54 mmol, (**A**) Si-ZnBA-3 150 mg, 2.0 MPa, 5.0 h; (**B**) Si-ZnBA-2 150 mg, 130 °C, 5.0 h; (**C**) Si-ZnBA-3 150 mg, 130 °C, 2.0 MPa; (**D**) 130 °C, 2.0 MPa, 5.0 h.