

Electronic Supplementary information for

Reengineering of the carbon-to-acetylene process featuring negative carbon emission

Miao Li^{a,b}, Hong Zhao^{a,*}, Siyuan Chen^a, Siyuan liu^a, Long Yan^c, Chen Hou^a, Biao Jiang^{a,*}

^a: Green Chemical Engineering Research Centre, Shanghai Advanced Research Institute,
Chinese Academy of Sciences, Shanghai 201210, China

^b: University of Chinese Academy of Sciences, Beijing 100049, China

^c: School of Chemistry and Chemical Engineering, Yulin University, Yulin 719000, China

*: Corresponding author: Email: zhaoh@sari.ac.cn, jiangb@sari.ac.cn

Content

Table S1 Thermodynamic initial temperature and theoretical mass loss* of possible reactions for BaC ₂ and CaC ₂ synthesis	2
Table S2 Mass balance of Ba before and after reaction at different temperature and reaction time.	2
Fig. S1 (a)The corresponding EDS mapping images of (a)reactants, heating products at 1150 °C, (c) at 1400 °C for 60 min, and (d) at 1550 °C for 30 min.....	2
Fig. S2 Pictures of reactant pellets and product pellets. (a) Reactant pellets. (b) Product pellets, BaC ₂ content: 91.4 wt%, experimental conditions: 1550 °C, 30 min.	3
Fig. S3 Solubility of Ca(OH)₂ and Ba(OH)₂ in water.	3
Fig. S4 (a) SEM images of recycled BaCO ₃ . (b) SEM images of fresh BaCO ₃	3

Table S1 Thermodynamic initial temperature and theoretical mass loss* of possible reactions for BaC₂ and CaC₂ synthesis

	Reaction	Theoretical initial temperature	Theoretical mass loss
BaC ₂ synthesis ¹	BaCO ₃ +C=BaO+2CO	1047°C	22.8 wt.%
	BaCO ₃ +4C=BaC ₂ +3CO	1242°C	34.2 wt.%
	BaCO ₃ =BaO+CO ₂	1558°C	18.0 wt.%
	BaO+3C=BaC ₂	1533°C	11.4 wt.%
CaC ₂ synthesis	CaCO ₃ =CaO+CO ₂	887°C	29.7 wt.%
	CaCO ₃ +C=CaO+2CO	--	37.8 wt.%
	C+CO ₂ =2CO	700°C	--

*Reactants contains 1 mol carbonate and 4 mol carbon were used as reactants

Table S2 Mass balance of Ba before and after reaction at different temperature and reaction time

	1400°C	1450°C	1500°C	1550°C
20 min	0.63	0.76	0.76	0.68
30 min	0.66	0.73	0.44	0.71
40 min	0.33	0.53	0.24	0.74
50 min	0.29	0.60	0.89	0.65
60 min	0.73	0.71	0.58	0.60

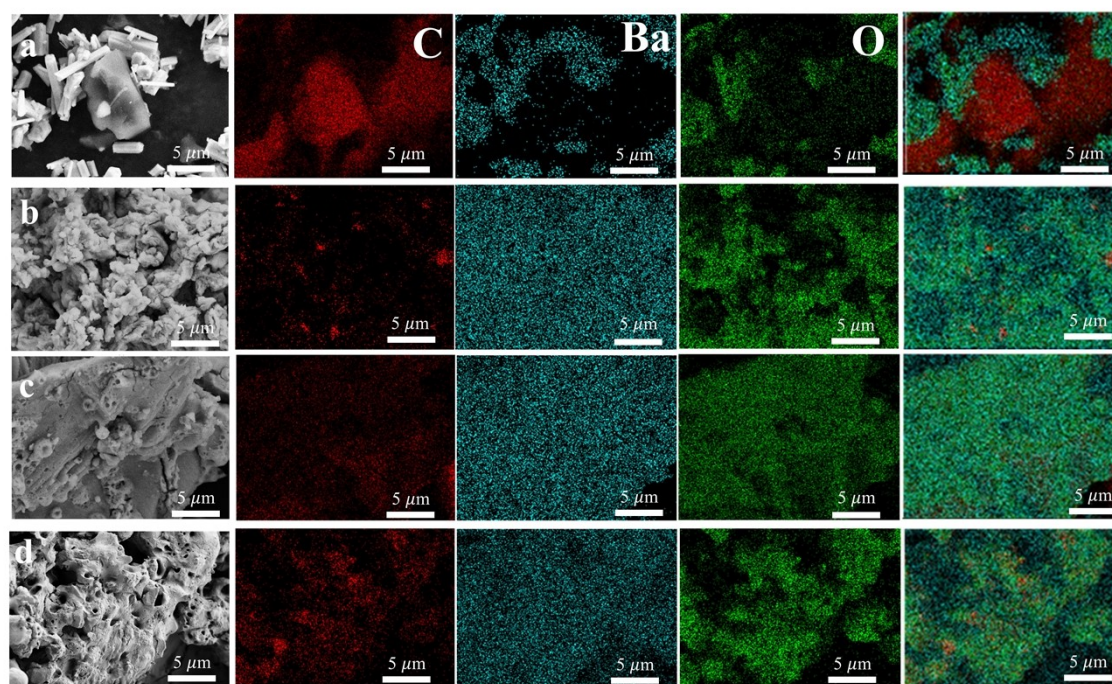


Fig. S1 (a)The corresponding EDS mapping images of (a)reactants, heating products at 1150 °C, (c) at 1400 °C for 60 min, and (d) at 1550 °C for 30 min.

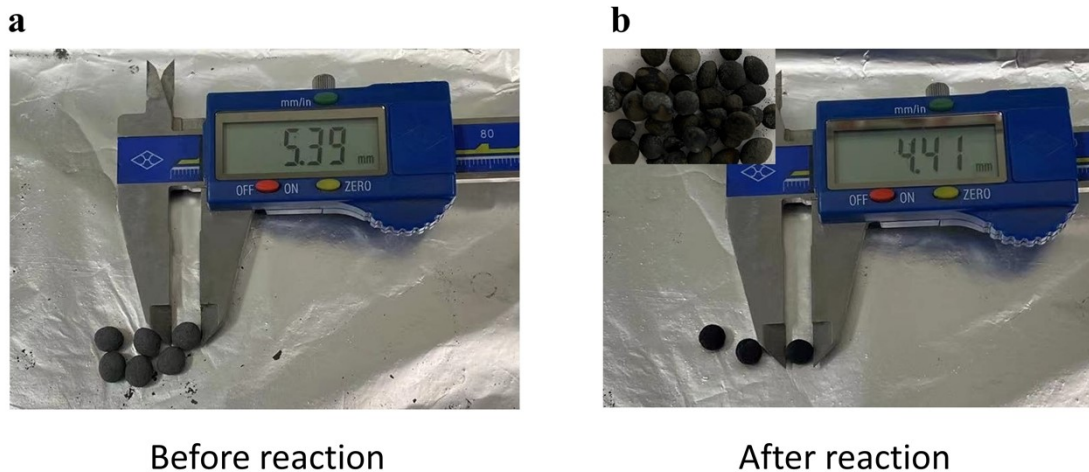


Fig. S2 Pictures of reactant pellets and product pellets. (a) Reactant pellets. (b) Product pellets, BaC₂ content: 91.4 wt%, experimental conditions: 1550 °C, 30 min.

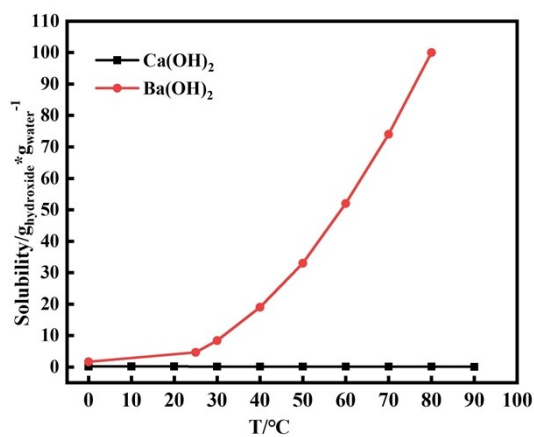


Fig. S3 Solubility of Ca(OH)₂ and Ba(OH)₂ in water.

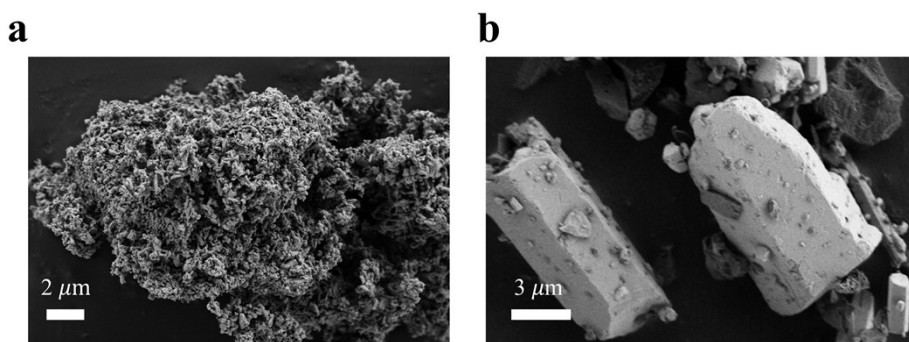


Fig. S4 (a) SEM images of recycled BaCO₃. (b) SEM images of fresh BaCO₃.

References

1. L. Miao, Z. Hong, J. Biao, C. Siyuan and Y. Long, *CIESC Journal*, 2022, **73**, 1908-1919.