Electronic Supplementary information for

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

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**Table S1** Thermodynamic initial temperature and theoretical mass loss* of possible reactions for BaC$_2$ and CaC$_2$ synthesis

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Theoretical initial temperature</th>
<th>Theoretical mass loss</th>
</tr>
</thead>
<tbody>
<tr>
<td>BaC$_2$ synthesis</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\text{BaCO}_3 + \text{C} = \text{BaO} + 2\text{CO}$</td>
<td>1047°C</td>
<td>22.8 wt.%</td>
</tr>
<tr>
<td>$\text{BaCO}_3 + 4\text{C} = \text{BaC}_2 + 3\text{CO}$</td>
<td>1242°C</td>
<td>34.2 wt.%</td>
</tr>
<tr>
<td>$\text{BaCO}_3 = \text{BaO} + \text{CO}_2$</td>
<td>1558°C</td>
<td>18.0 wt.%</td>
</tr>
<tr>
<td>$\text{BaO} + 3\text{C} = \text{BaC}_2$</td>
<td>1533°C</td>
<td>11.4 wt.%</td>
</tr>
<tr>
<td>CaC$_2$ synthesis</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\text{CaCO}_3 = \text{CaO} + \text{CO}_2$</td>
<td>887°C</td>
<td>29.7 wt.%</td>
</tr>
<tr>
<td>$\text{CaCO}_3 + \text{C} = \text{CaO} + 2\text{CO}$</td>
<td>--</td>
<td>37.8 wt.%</td>
</tr>
<tr>
<td>$\text{C} + \text{CO}_2 = 2\text{CO}$</td>
<td>700°C</td>
<td>--</td>
</tr>
</tbody>
</table>

*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

<table>
<thead>
<tr>
<th></th>
<th>1400°C</th>
<th>1450°C</th>
<th>1500°C</th>
<th>1550°C</th>
</tr>
</thead>
<tbody>
<tr>
<td>20 min</td>
<td>0.63</td>
<td>0.76</td>
<td>0.76</td>
<td>0.68</td>
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<tr>
<td>30 min</td>
<td>0.66</td>
<td>0.73</td>
<td>0.44</td>
<td>0.71</td>
</tr>
<tr>
<td>40 min</td>
<td>0.33</td>
<td>0.53</td>
<td>0.24</td>
<td>0.74</td>
</tr>
<tr>
<td>50 min</td>
<td>0.29</td>
<td>0.60</td>
<td>0.89</td>
<td>0.65</td>
</tr>
<tr>
<td>60 min</td>
<td>0.73</td>
<td>0.71</td>
<td>0.58</td>
<td>0.60</td>
</tr>
</tbody>
</table>

**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, BaC$_2$ 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 BaCO$_3$. (b) SEM images of fresh BaCO$_3$.

References