Supporting information for

Theoretical and experimental studies of high efficient all-solid Z-scheme TiO$_2$-TiC/g-C$_3$N$_4$ for photocatalytic CO$_2$ reduction via dry reforming of methane

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Figure S1. The diagram of the experimental device for photocatalytic CO$_2$ in the presence of CH$_4$. 
Figure S2. (a) N$_2$ physisorption isotherms and corresponding pore size distribution curves (inset) and (b) The CO$_2$ adsorption capacity of g-C$_3$N$_4$ and (25)TiO$_2$-TiC/g-C$_3$N$_4$(400).
Table S1. BET specific surface area and total pore volume of g-C\textsubscript{3}N\textsubscript{4} and (25)TiO\textsubscript{2}-TiC/g-C\textsubscript{3}N\textsubscript{4}(400).

<table>
<thead>
<tr>
<th>Parameter</th>
<th>g-C\textsubscript{3}N\textsubscript{4}</th>
<th>(25)TiO\textsubscript{2}-TiC/g-C\textsubscript{3}N\textsubscript{4}(400)</th>
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<tbody>
<tr>
<td>Specific surface area (m\textsuperscript{2}/g)</td>
<td>16.920</td>
<td>21.503</td>
</tr>
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<td>Total pore volume (cm\textsuperscript{3}/g)</td>
<td>0.087</td>
<td>0.078</td>
</tr>
<tr>
<td></td>
<td>Level 1</td>
<td>Level 2</td>
</tr>
<tr>
<td>--------</td>
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<td>---------</td>
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<tr>
<td>$F_A$: Absolute pressure (kPa)</td>
<td>10</td>
<td>20</td>
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<tr>
<td>$F_B$: CH$_4$ to CO$_2$ ratio</td>
<td>2:1</td>
<td>1:1</td>
</tr>
<tr>
<td>$F_C$: TiC loading (mg)</td>
<td>15</td>
<td>20</td>
</tr>
<tr>
<td>$F_D$: Calcination temperature (℃)</td>
<td>350</td>
<td>400</td>
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Table S3. The detailed experimental conditions of four factors and four levels (L₁₆(4⁴)) orthogonal test.

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<tr>
<th>Experiment Numbers</th>
<th>F₁: pressure (kPa)</th>
<th>F₂: mole ratio of CH₄: CO₂</th>
<th>F₃: Loading of TiC (mg)</th>
<th>F₄: calcination temperature (℃)</th>
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<td>Experiment Numbers</td>
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<td>CO (μmol)</td>
<td>TOF_{H₂} (μmol g⁻¹ h⁻¹)</td>
<td>TOF_{CO} (μmol g⁻¹ h⁻¹)</td>
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Figure S3. X-ray diffraction patterns of (25)TiO$_2$-TiC/g-C$_3$N$_4$(350), (25)TiO$_2$-TiC/g-C$_3$N$_4$(400), (25)TiO$_2$-TiC/g-C$_3$N$_4$(450), (25)TiO$_2$-TiC/g-C$_3$N$_4$(500).
Figure S4. SEM patterns of (25)TiO\textsubscript{2}-TiC/g-C\textsubscript{3}N\textsubscript{4}(350), (25)TiO\textsubscript{2}-TiC/g-C\textsubscript{3}N\textsubscript{4}(400), (25)TiO\textsubscript{2}-TiC/g-C\textsubscript{3}N\textsubscript{4}(450), (25)TiO\textsubscript{2}-TiC/g-C\textsubscript{3}N\textsubscript{4}(500).
Figure S5. (a) UV−vis absorption spectra and (b) PL emission spectra of TiO$_2$-TiC/g-C$_3$N$_4$ calcinating under different temperature.
Figure S6. Illustrations of (a) $2 \times \sqrt{3}$ relaxed rectangular g-C$_3$N$_4$ monolayer; (b) original g-C$_3$N$_4$ monolayer; (c) TiO$_2$ (101) surface; (d) TiO$_2$/g-C$_3$N$_4$ heterostructure. Deep gray, blue, red, and light gray balls represent C, N, O and Ti atoms, respectively; this notation is used throughout the paper.
Figure S7. Illustrations of (a) TiO$_2$-TiC/g-C$_3$N$_4$ heterostructure with TiC on the TiO$_2$ side; (b) TiO$_2$-TiC/g-C$_3$N$_4$ heterostructure with TiC between TiO$_2$ and g-C$_3$N$_4$; (c) TiO$_2$-TiC/g-C$_3$N$_4$ heterostructure with (TiC)$_3$ on the TiO$_2$ side; (d) TiO$_2$-TiC/g-C$_3$N$_4$ heterostructure with (TiC)$_3$ between TiO$_2$ and g-C$_3$N$_4$. 
Figure S8. Density of state (DOS) of four structures in Figure S7. (a) – (d) correspond to structures (a) – (d) in Figure S7.
Figure S9. Electrostatic potentials and density of states of (ab) the monolayer $g\text{-C}_3N_4$; (cd) TiO$_2$(101) surface. The DOS Figures in this study are plotted using DosPlotter module in Pymatgen python package (https://pymatgen.org/).
Figure S10. Calculated optical adsorption spectra of TiO$_2$(101), TCC-a, and TCC-b.