Plasma-photocatalytic conversion of CO$_2$ at low temperatures: Understanding the synergistic effect of plasma-catalysis

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1. Thermodynamic equilibrium calculation

The thermodynamic equilibrium calculation of CO₂ conversion was carried out using the method based on the minimization of Gibbs free energy in a closed system. The main gas products are CO and O₂. No O₃ was detected in the present experiment. We can see that CO₂ begins to decompose into CO and O₂ near 2000 K and the conversion of CO₂ is very low (< 1%). Reasonable conversion of CO₂ (~60%) can be obtained at an extraordinarily high temperature (3000-3500K), which leads to the high energy cost for thermal conversion of CO₂.

![Thermodynamic equilibrium calculation of CO₂ conversion as a function of temperature](image1)

(a)

![CO₂ conversion (%) vs. temperature](image2)

(b)

Fig. SI1 Thermodynamic equilibrium calculation of CO₂ conversion as a function of
operating temperature at 1 atm (without plasma) (a) gas composition vs. temperature; (b) CO$_2$ conversion vs. temperature.

2. **Mean Electric field and electron energy**

The average electric field of the discharge (breakdown voltage/electrode gap) and the mean electron energy for the three different experimental conditions are calculated through Lissajous figure and BOLSIG$^+$ code based on electron energy distribution function (EEDF), respectively[1, 2] and the corresponding results are shown in Fig. SI2.
Fig. SI2 Average electric field (a) and mean electron energy (b) of the CO$_2$ DBD with and without catalyst.

3. Catalyst characterization

XRD patterns of the catalyst samples are plotted in Figure SI3. BaTiO$_3$ has the tetragonal phase [3], which can be approved by the peaks at $2\theta = 22.14^\circ$, 31.61$^\circ$, 39.00$^\circ$, 45.37$^\circ$, 51.00$^\circ$, 56.32$^\circ$, 65.94$^\circ$ (JCPDS 05-0626), while the fresh TiO$_2$ shows a crystal structure of anatase, as evidenced by X-ray reflections at $2\theta = 25.24^\circ$, 36.94$^\circ$, 37.82$^\circ$, 38.56$^\circ$, 48.04$^\circ$, 53.96$^\circ$, 55.00$^\circ$, 62.69$^\circ$, 68.76$^\circ$ (JCPDS 84-1286)[4].

![Fig. SI3 XRD patterns of the fresh catalysts.](image)

Reference

