

Table S1: Relationship between surface strategies and photocatalytic CO₂ reduction properties in 2D materials (Green rectangles represent applicable strategies)

| <i>CO₂ reduction</i> <i>Surface Strategies</i> | <i>CO₂ adsorption</i> | <i>Light utilization</i> | <i>Carriers separation</i> | <i>Carriers Transfer</i> | <i>CO₂ Activation</i> | <i>Selectivity</i> | <i>Products desorption</i> |
|--|----------------------------------|--------------------------|----------------------------|--------------------------|----------------------------------|--------------------|----------------------------|
| <i>Defect Engineering</i> | Green | Green | Green | Green | Green | | |
| <i>Heteroatom Engineering</i> | | Green | Green | | | Green | |
| <i>Composite</i> | Green | | Green | | Green | Green | |
| <i>Surface molecular functionalization</i> | Green | | | | | | |

Table S2: Relationship between surface strategies and electrocatalytic CO₂ reduction properties in 2D materials (Green rectangles represent applicable strategies)

| <i>CO₂ reduction</i> <i>Surface Strategies</i> | <i>CO₂ adsorption</i> | <i>Conductivity</i> | <i>Activation barrier</i> | <i>Intermediate Stabilization</i> | <i>Selectivity</i> | <i>Products desorption</i> |
|--|----------------------------------|---------------------|---------------------------|-----------------------------------|--------------------|----------------------------|
| <i>Defect Engineering</i> | Green | Green | Green | Green | Green | |
| <i>Heteroatom Engineering</i> | | | | | Green | |
| <i>Composite</i> | | Green | Green | Green | Green | |
| <i>Surface molecular functionalization</i> | Green | | | | | Green |
| <i>Surface alloy</i> | | | | Green | | Green |