

# Probing the surface chemistry of CO<sub>2</sub> by qPlus-AFM

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Carbon dioxide (CO<sub>2</sub>) chemistry has attracted an increasing interest in recent years, motivated by the carbon-neutral fuel cycle. However, CO<sub>2</sub> is highly inert and the activation of CO<sub>2</sub> is difficult and costly. Many research works have evidenced the crucial role of alkali metal cations on the activation and conversion of CO<sub>2</sub>. One of the key reasons is that the metal cations at the interface could stabilize the reaction intermediates, but the atomic-scale characterization of metal-CO<sub>2</sub> complexes during CO<sub>2</sub> activation is lacking.

Using qPlus based noncontact atomic force microscopy (nc-AFM), we directly visualized the atomic structure of isolated CO<sub>2</sub> molecule on Cu(110)-(2 × 1)-O surface. Then we explored how the alkali cations on copper surfaces activate carbon dioxide molecules. At the initial step, we observed the aggregation of alkali cations to stabilize the activated bending CO<sub>2</sub> molecule through cation coupled electron transfer on both Cu(111) and Cu(100) surfaces. More interestingly, the activated CO<sub>2</sub> molecules could further transform into oxalate through carbon-carbon coupling on Cu(100) surface, in which the oxalate ions are stabilized by alkali cation tetramers. Increasing the pressure of carbon dioxide, 2D alkali carbonate films formed on Cu(111) due to the disproportionation reaction between CO<sub>2</sub> molecules. Our findings directly visualized the promoting role of alkali cations on the activation of carbon dioxide on copper and revealed the electron transfer mechanism.

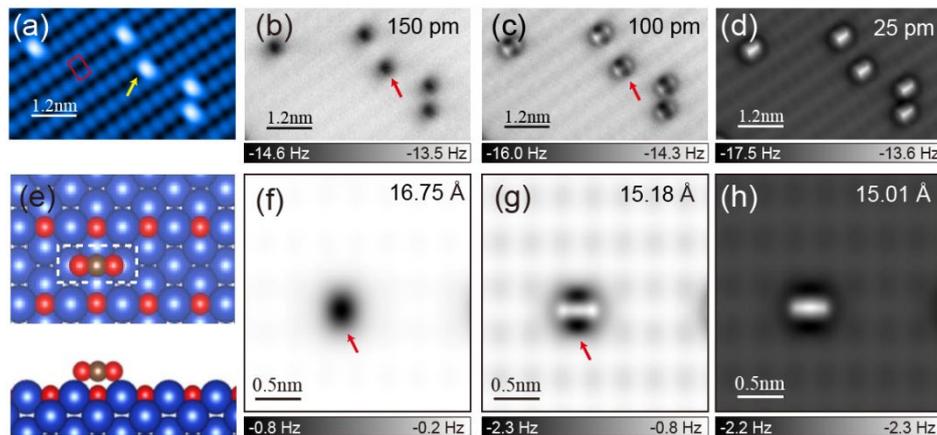


Fig. 1. High resolution AFM images of CO<sub>2</sub> molecules on Cu(110)-(2 × 1)-O surface.