

Abstract Submitted  
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**Interaction of CO<sub>2</sub> with Oxygen Adatoms on Rutile TiO<sub>2</sub>(110) Surface**<sup>1</sup> XIAO LIN, YEOHOON YOON, ZHENJUN LI, ZHI-TAO WANG, BRUCE D. KAY, IGOR LYUBINETSKY, ROGER ROUSSEAU, ZDENEK DOHNALEK, Pacific Northwest National Laboratory — On TiO<sub>2</sub>(110), oxygen vacancies ( $V_O$ 's) act as the primary catalytic sites and as such they have been extensively investigated. However, only a few studies have been reported about the interactions of adsorbates with oxygen adatoms ( $O_a$ 's) that are created by O<sub>2</sub> dissociation in  $V_O$ 's. Here, we report a combined scanning tunneling microscopy (STM) / density functional theory (DFT) study of CO<sub>2</sub> on bare and  $O_a$  covered TiO<sub>2</sub>(110). STM images of TiO<sub>2</sub>(110) surfaces obtained before and after in-situ dose at ~50 K show that CO<sub>2</sub> molecules preferentially adsorb next to  $O_a$ 's forming CO<sub>2</sub>/ $O_a$  complexes. Temperature dependent studies further reveal that the CO<sub>2</sub> binding energy next to  $O_a$ 's is similar to that on  $V_O$ 's. Additional CO<sub>2</sub> molecules are found to diffuse rapidly along the Ti row between two CO<sub>2</sub>/ $O_a$  complexes. Due to the slow STM sampling rate the images display a time average of all CO<sub>2</sub> binding configurations on the Ti rows and reveal differences in the populations found on ideal Ti sites and Ti sites next to  $V_O$ 's.

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