

Electronic supplementary information (ESI)

**Enhanced adsorption of CO₂ at steps of ultrathin ZnO: the importance of
Zn-O geometry and coordination**

Xingyi Deng^{1,2,*}, Dan C. Sorescu¹, Junseok Lee^{1,2}

¹National Energy Technology Laboratory (NETL), United States Department of Energy, P.O. Box
10940, Pittsburgh, Pennsylvania 15236, United States, ²AECOM, P.O. Box 618, South Park,
Pennsylvania 15129, United States

Corresponding Author E-mail: Xingyi.Deng@NETL.DOE.GOV

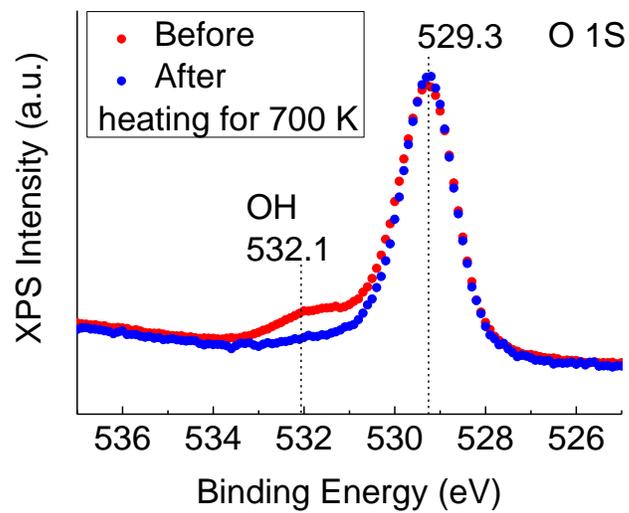


Fig. S1 O 1s XP spectra of as-prepared 1.7 MLE ZnO(L2-L3) and after heating to 700 K, showing the removal of hydroxyls.

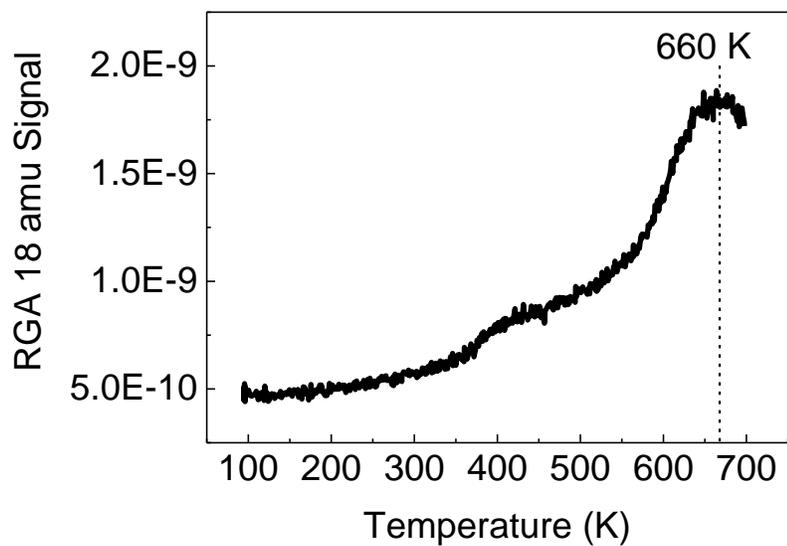


Fig. S2 TPD spectrum of H₂O (m/z = 18) from as-prepared 1.7 MLE ZnO(L2-L3), showing the hydroxyl removal via recombinative desorption as water occurring at T = 660 K (heating rate 2 K/s).

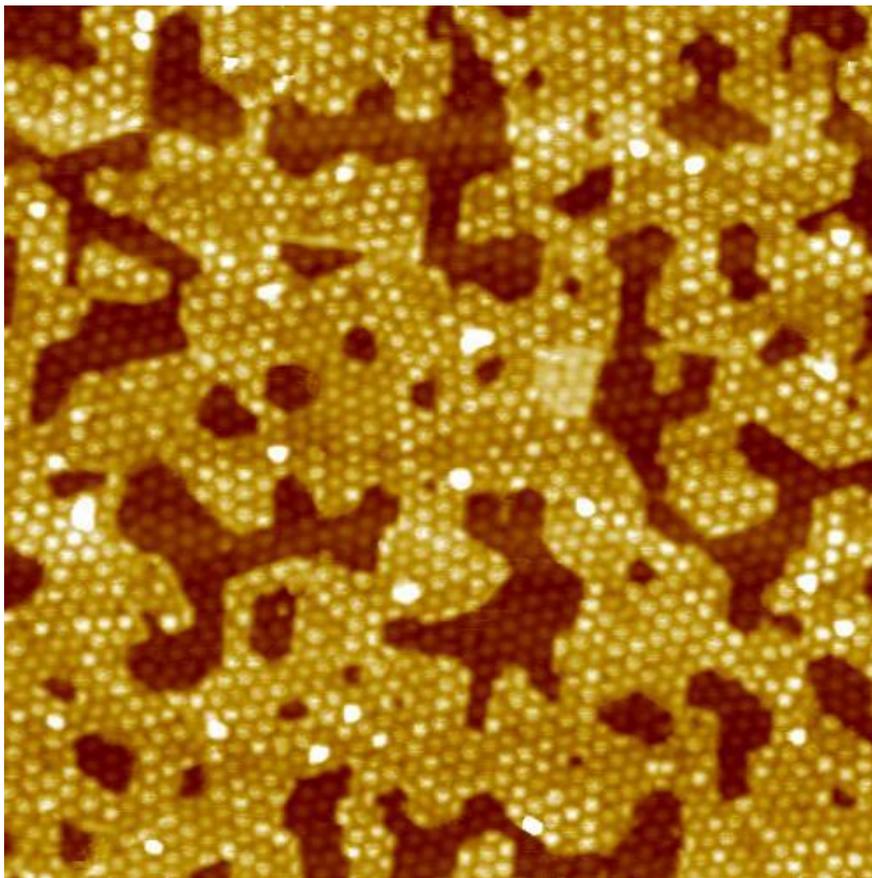


Fig. S3 STM image of 2.3 MLE ZnO(L2-L3) ($100 \times 100 \text{ nm}^2$, $V = 1.5 \text{ V}$, $I = 50 \text{ pA}$).

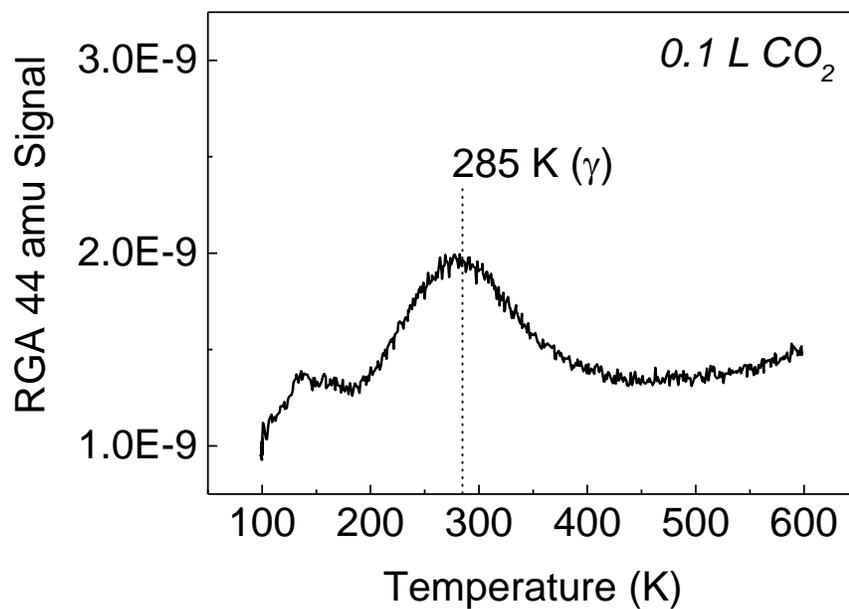


Fig. S4 TPD spectrum of CO₂ ($m/z = 44$) from 2.3 MLE ZnO(L2-L3) following the CO₂ exposure of 0.1 L ($1 \text{ L} = 1.33 \times 10^{-6} \text{ mbar}\cdot\text{s}$) at $T = 100 \text{ K}$ (heating rate 2 K/s).