Electronic supplementary information (ESI)

Enhanced adsorption of CO$_2$ at steps of ultrathin ZnO: the importance of Zn-O geometry and coordination

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

$^1$National Energy Technology Laboratory (NETL), United States Department of Energy, P.O. Box 10940, Pittsburgh, Pennsylvania 15236, United States, $^2$AECOM, 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 H$_2$O (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 × 100 nm², V = 1.5 V, I = 50 pA).
Fig. S4 TPD spectrum of CO$_2$ (m/z = 44) from 2.3 MLE ZnO(L2-L3) following the CO$_2$ exposure of 0.1 L (1 L = 1.33 × 10$^{-6}$ mbar·s) at T = 100 K (heating rate 2 K/s).