SUPPORTING INFORMATION

Ethanol Sensing Mechanism of ZnO Nanorods Revealed by DRIFT Spectroscopy and DFT Calculations

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A. ZnO single crystals

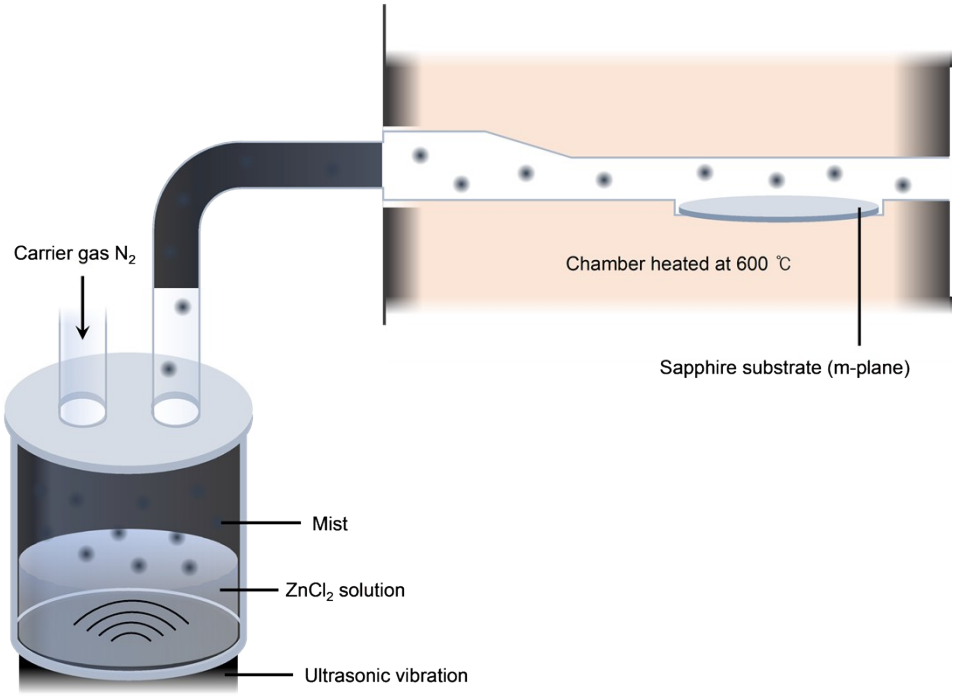

Fig. S1 Schematic diagram of the mist chemical vapor deposition setup.

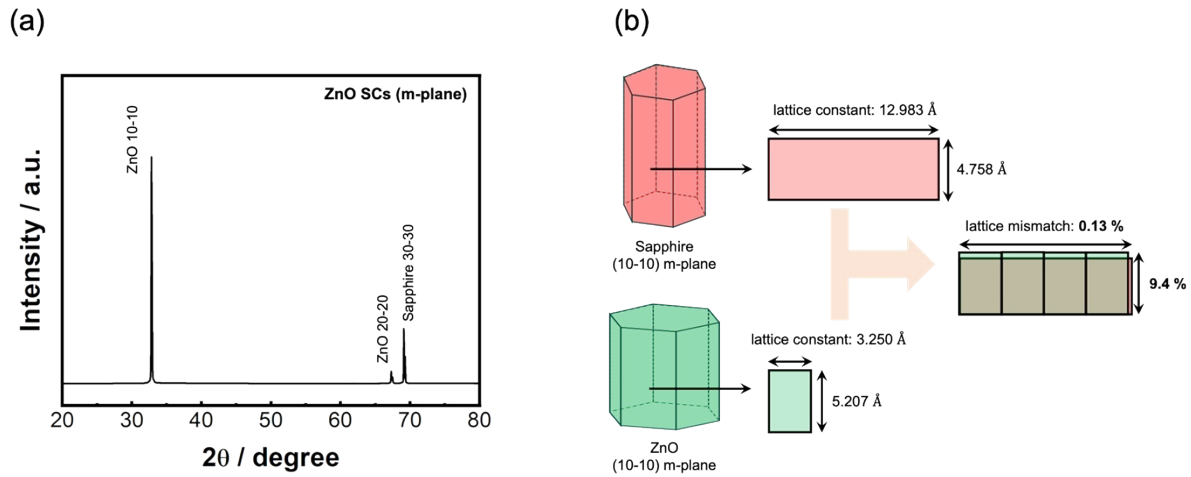

Fig. S2 (a) XRD pattern of the sensing layer with *m*-plane ZnO single crystals. (b) Lattice mismatch between sapphire and ZnO with respect to their (10-10) plane.

B. Geometry of the (10-10) plane of ZnO from DFT calculations

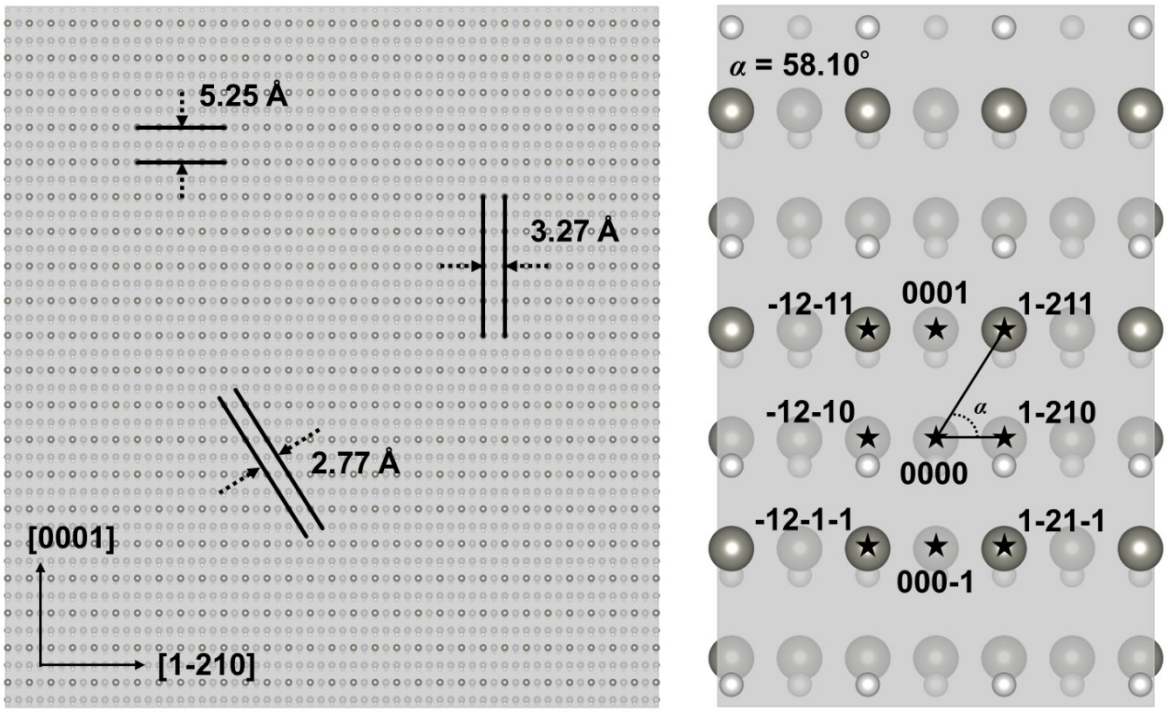

Fig. S3 (a) Interatomic distances in the (10-10) plane of ZnO. (b) Planes intersecting the (10-10) plane of ZnO.

C. DRIFTS and gas cell measurements at 100–250 °C

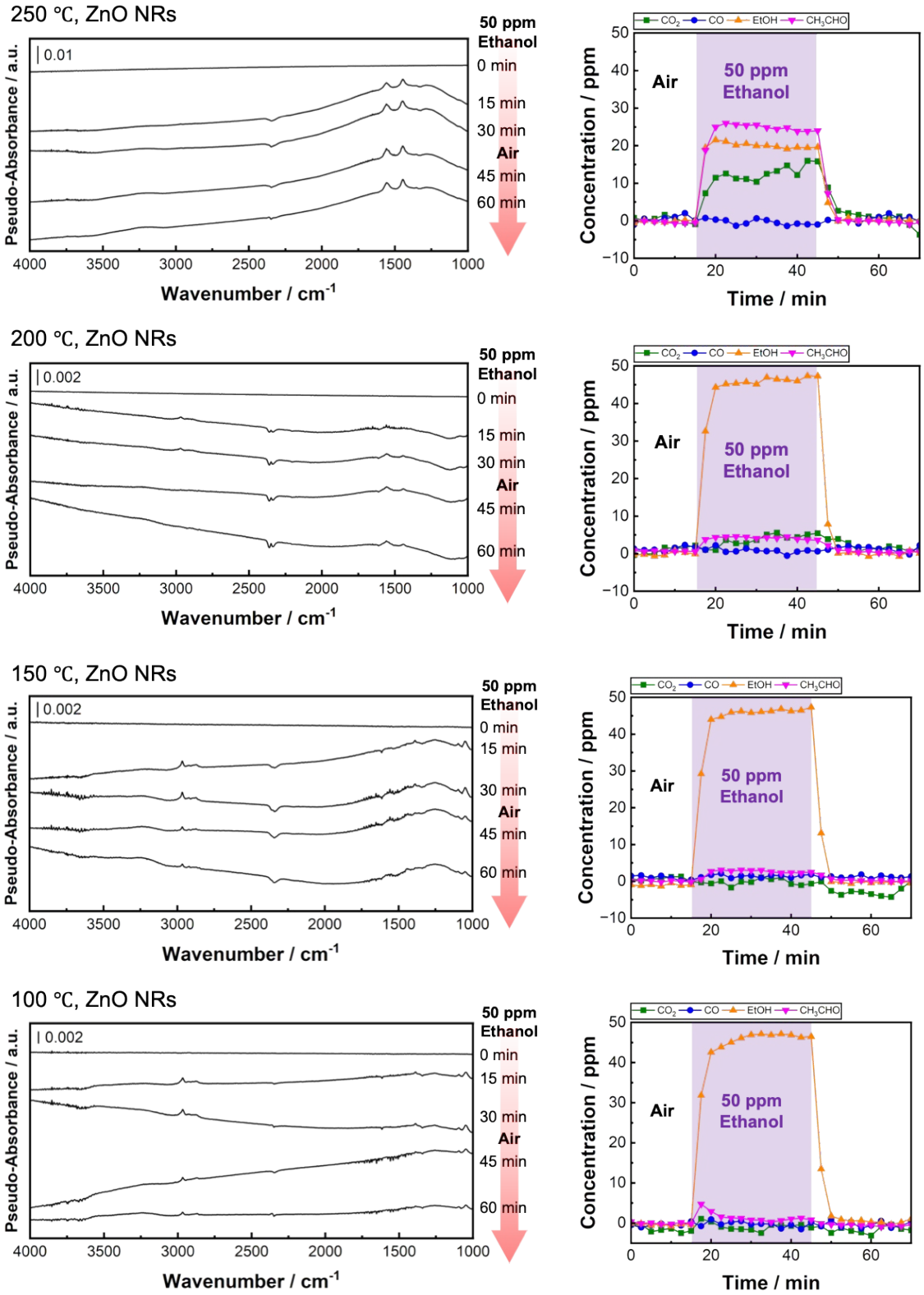

Fig. S4 Absorbance spectra of ZnO nanorods NRs (left plots) and concentration of outlet gas (right plots) under 50 ppm ethanol exposure for 30 minutes then air exposure for another 30 minutes at different temperatures.

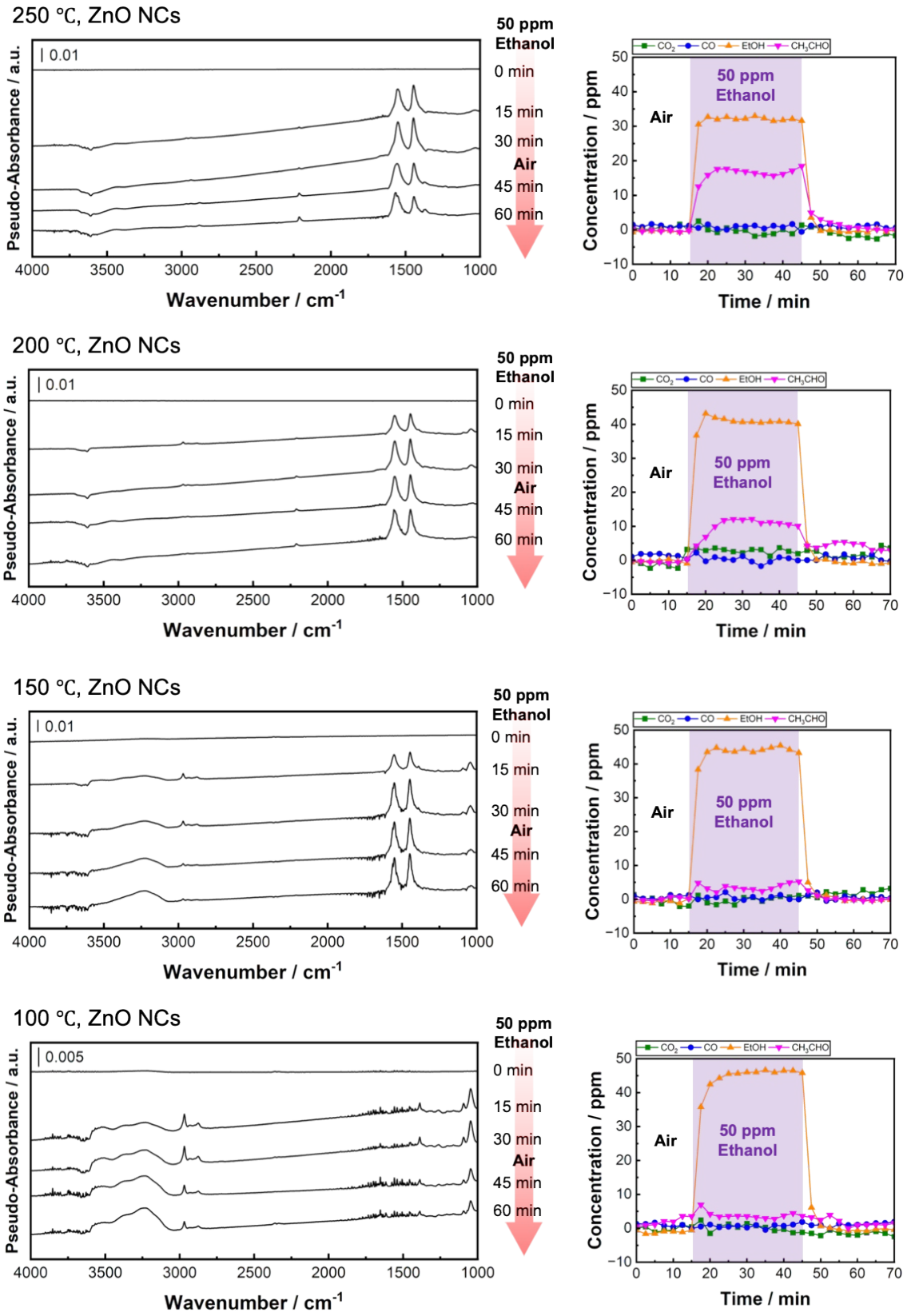

Fig. S5 Absorbance spectra of ZnO nanocrystals NCs (left plots) and concentration of outlet gas (right plots) under 50 ppm ethanol exposure for 30 minutes then air exposure for another 30 minutes at different temperatures.

D. Integrated local density of states of ethoxide and acetaldehyde adsorbed on the ZnO (10-10) surface

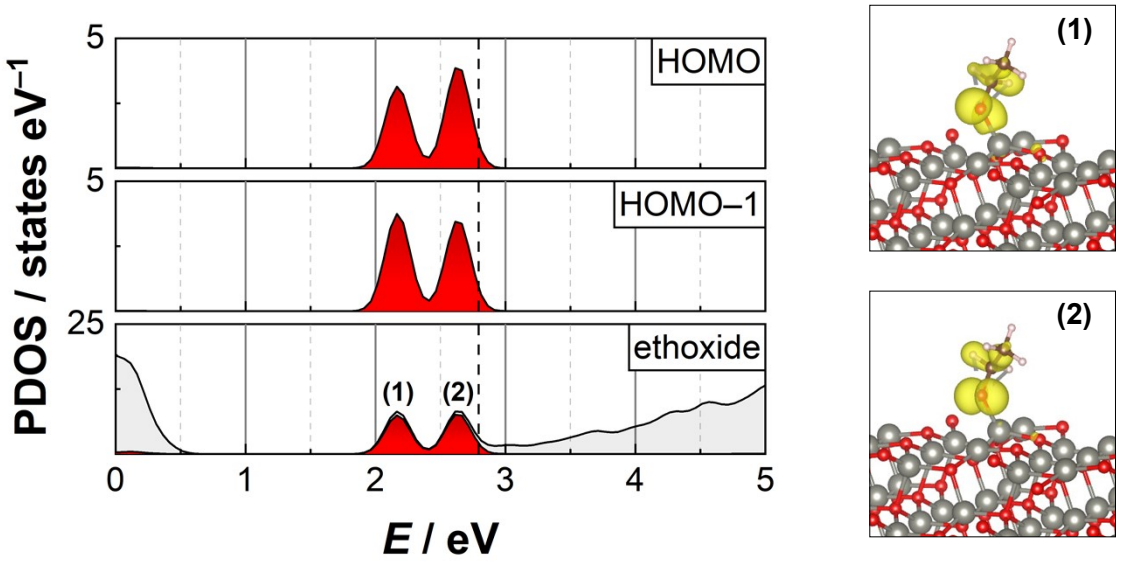

Fig. S6 Integrated local density of states of ZnO with an adsorbed ethoxide (plots on the left) and visualization of the ethoxide-surface interaction at the states within the band gap of ZnO (images on the right)

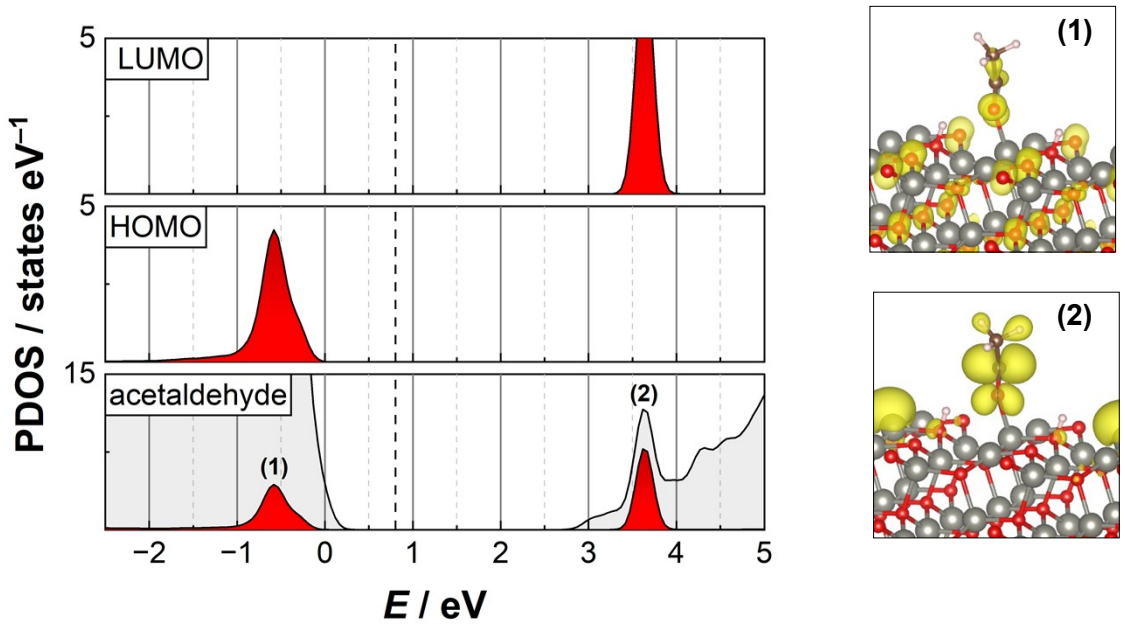

Fig. S7 Integrated local density of states of ZnO with an adsorbed acetaldehyde (plots on the left) and visualization of the acetaldehyde-surface interaction at the states within the band gap of ZnO (images on the right)

1 H. Tanoue, T. Taniguchi, S. Wada, S. Yamamoto, S. Nakamura, Y. Naka, H. Yoshikawa, M. Munekata, S. Nagaoka and Y. Nakamura, *Appl. Phys. Express*, , DOI:10.7567/APEX.8.125502.