Electronic Supplementary Information

for

Investigations of water-induced polar facet stabilization mechanism in ZnO nanoplates with ^1H NMR spectroscopy

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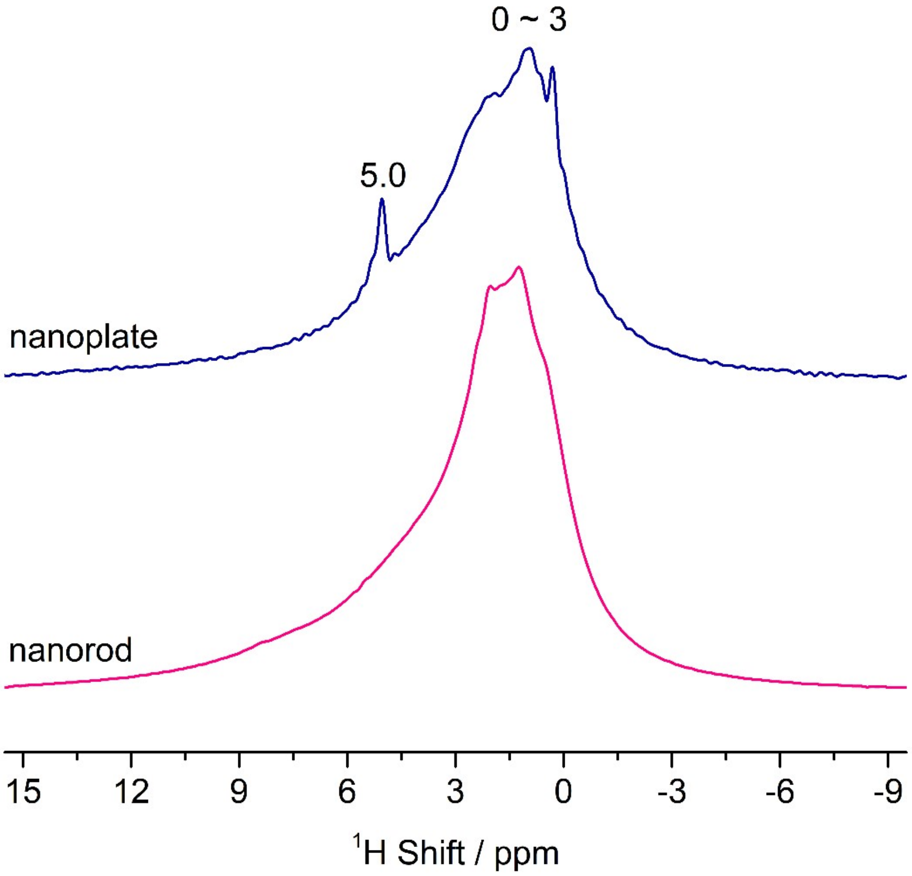

Figure S1. The comparison for ^{1}H NMR spectra of ZnO nanorods and ZnO nanoplates after vacuum dried at room temperature. Recycle delays of 5 s were used and 64 scans were collected for each NMR spectrum.

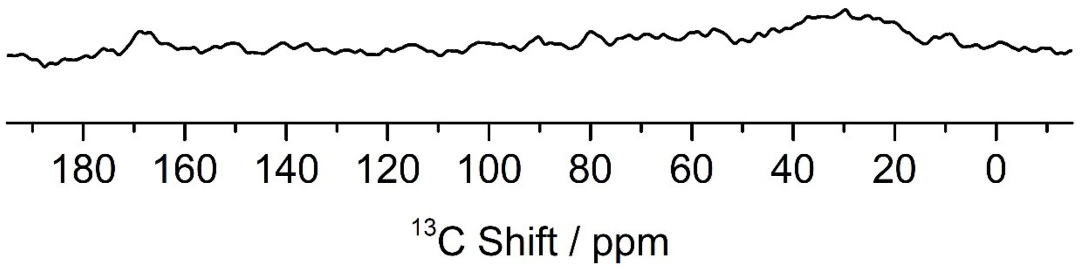

Figure S2. ^{13}C CP/MAS spectrum of ZnO nanoplates after washing and calcining procedures. The optimized contact time of 2000 μs and recycle delay of 5 s were used and 8000 acquisitions were accumulated for the spectrum.

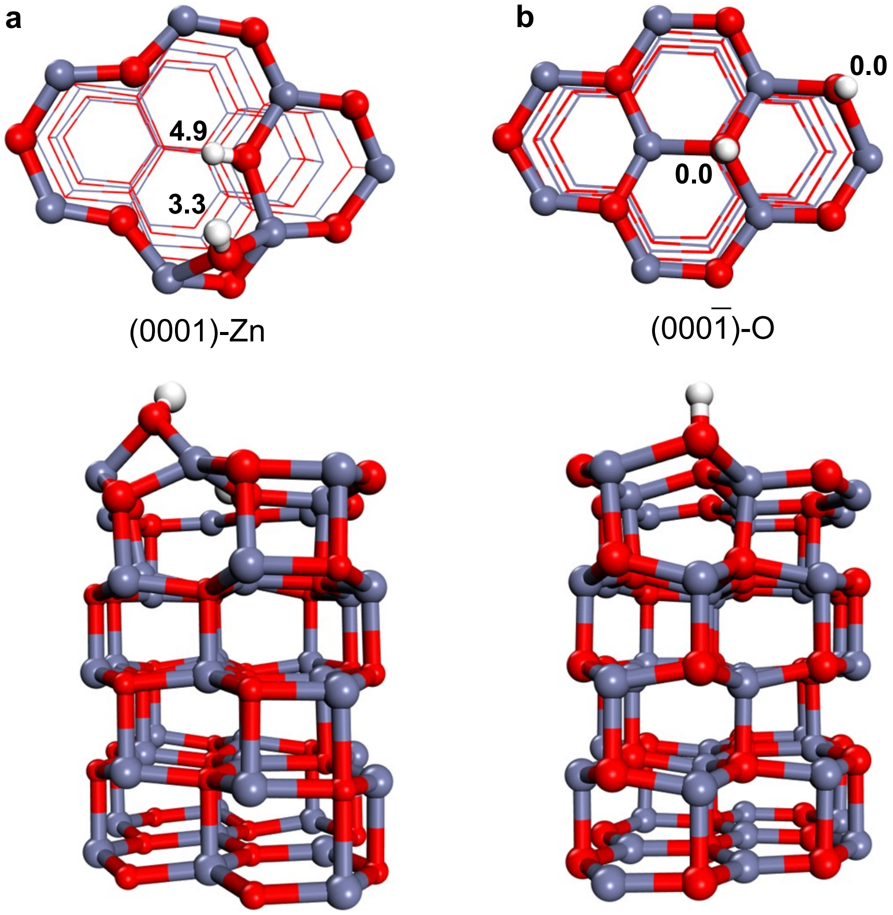

Figure S3. Calculated structures of ZnO nanoplates for water dissociation at Zn vacancy on polar Zn-terminated surface and at O vacancy on polar O-terminated surface, respectively, and corresponding chemical shifts for surface hydrogen species. Top: top view; bottom: side view. Gray, red and white spheres represent Zn, O and H atoms, respectively.

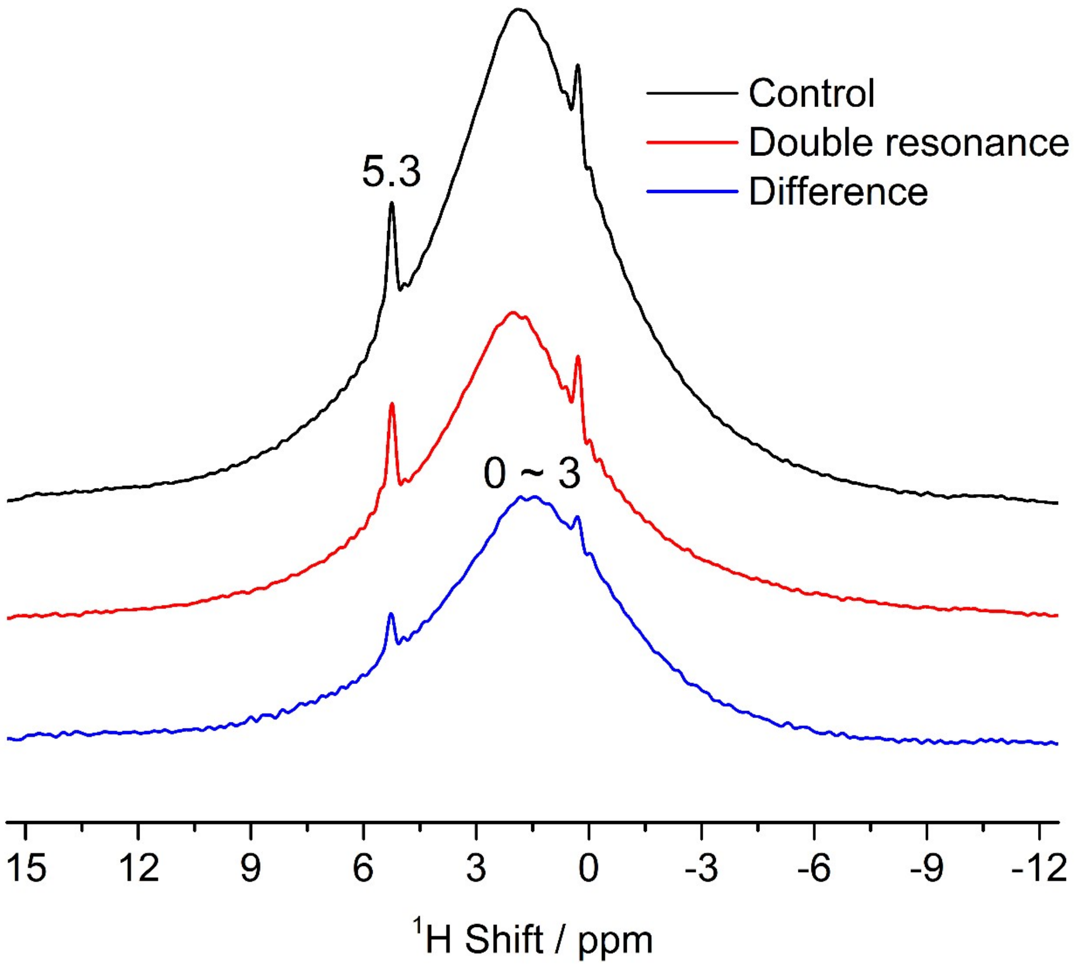

Figure S4. ^{1}H-^{17}O TRAPDOR NMR spectra of ZnO nanoplates. ^{17}O irradiation time: 0.2 ms; MAS rate: 5 kHz; recycle delay: 2 s; ^{17}O irradiation radio frequency (RF) field strength: 64 kHz. The difference spectrum is obtained by subtracting the double resonance spectrum from the control spectrum.

^{1}H-^{17}O transfer of population in double resonance (TRAPDOR) NMR experiments provide further evidences for spectral assignments.[1] TRAPDOR NMR spectra with a short ^{17}O irradiation time of about 0.2 ms are shown in Figure S4. The difference spectrum shows a broad peak at 0 ~ 3 ppm and a narrow peak at 5.3 ppm, implying relatively short H-O distances are involved for these hydrogen sites. Combined with discussions in Fig. 2 and our previous work in ZnO nanorods,[2] the broad peak at 0 ~ 3 ppm can be ascribed to hydroxyl groups and/or adsorbed water.

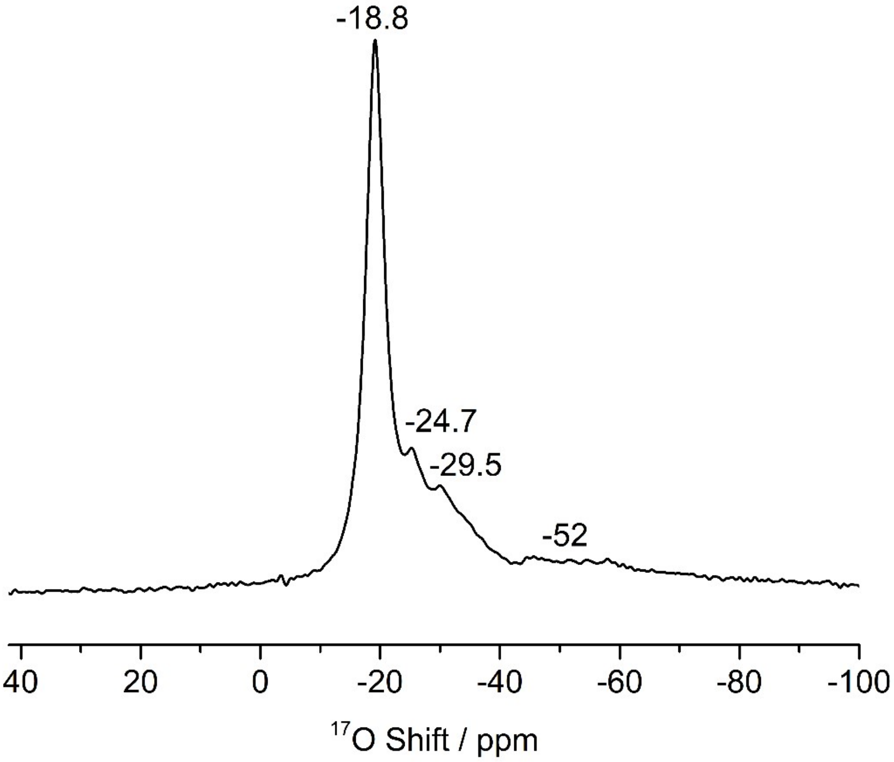

Figure S5. ^{17}O NMR spectra of ZnO nanoplates labeled with $H_2{}^{17}O$. A recycle delay of 5 s and 30° pulse of 1.2 μs were used and 2000 scans were collected for this spectrum.

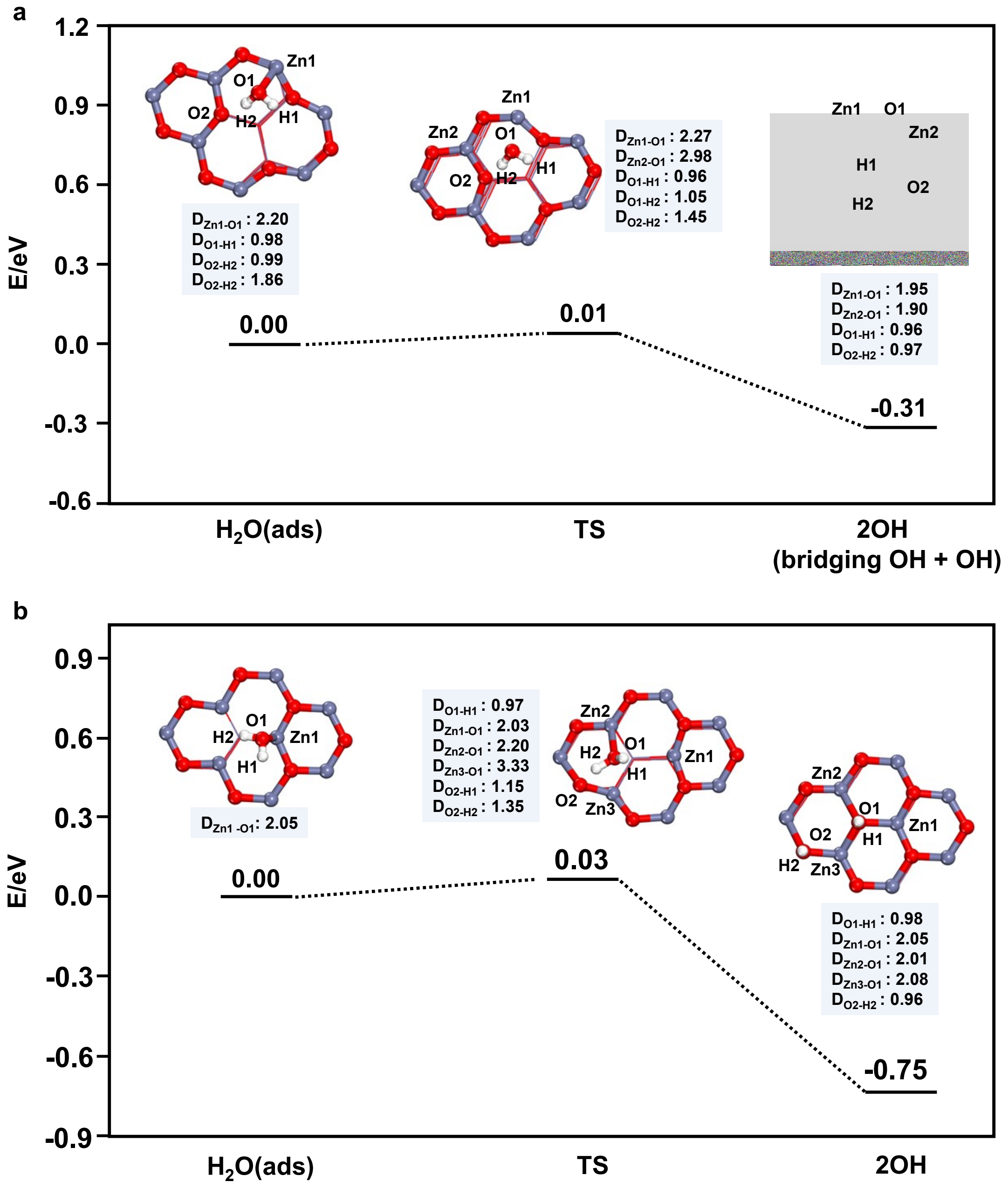

Figure S6. Calculated energy profiles for the dissociation of water at (a) Zn vacancy on (0001)-Zn surface of ZnO, and at (b) O vacancy on (000$\bar{1}$)-O surface. The distances are given in Å. "TS" represents transition states. Gray, red and white spheres represent Zn, O and H atoms, respectively.

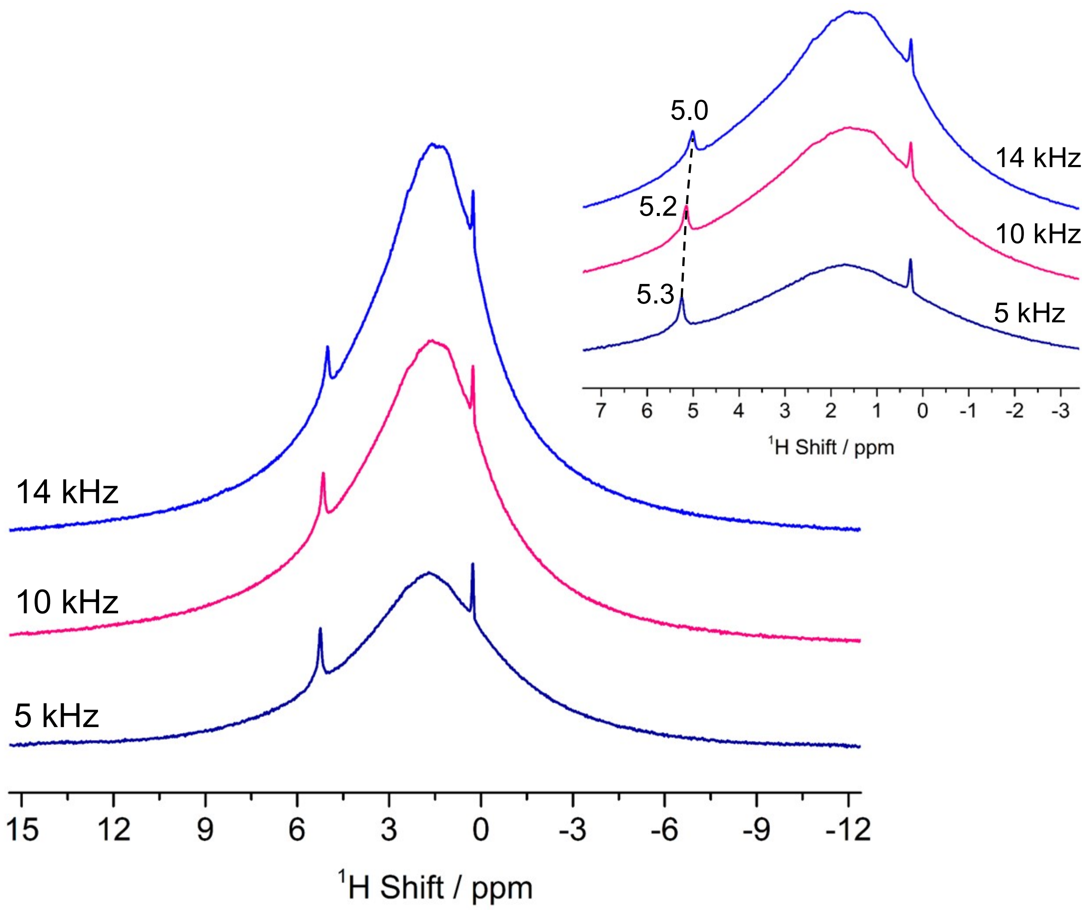

Figure S7. ^{1}H NMR spectra of ZnO nanoplates obtained under different spinning frequency. Recycle delays of 5 s were used and 64 scans were collected for each NMR spectrum.

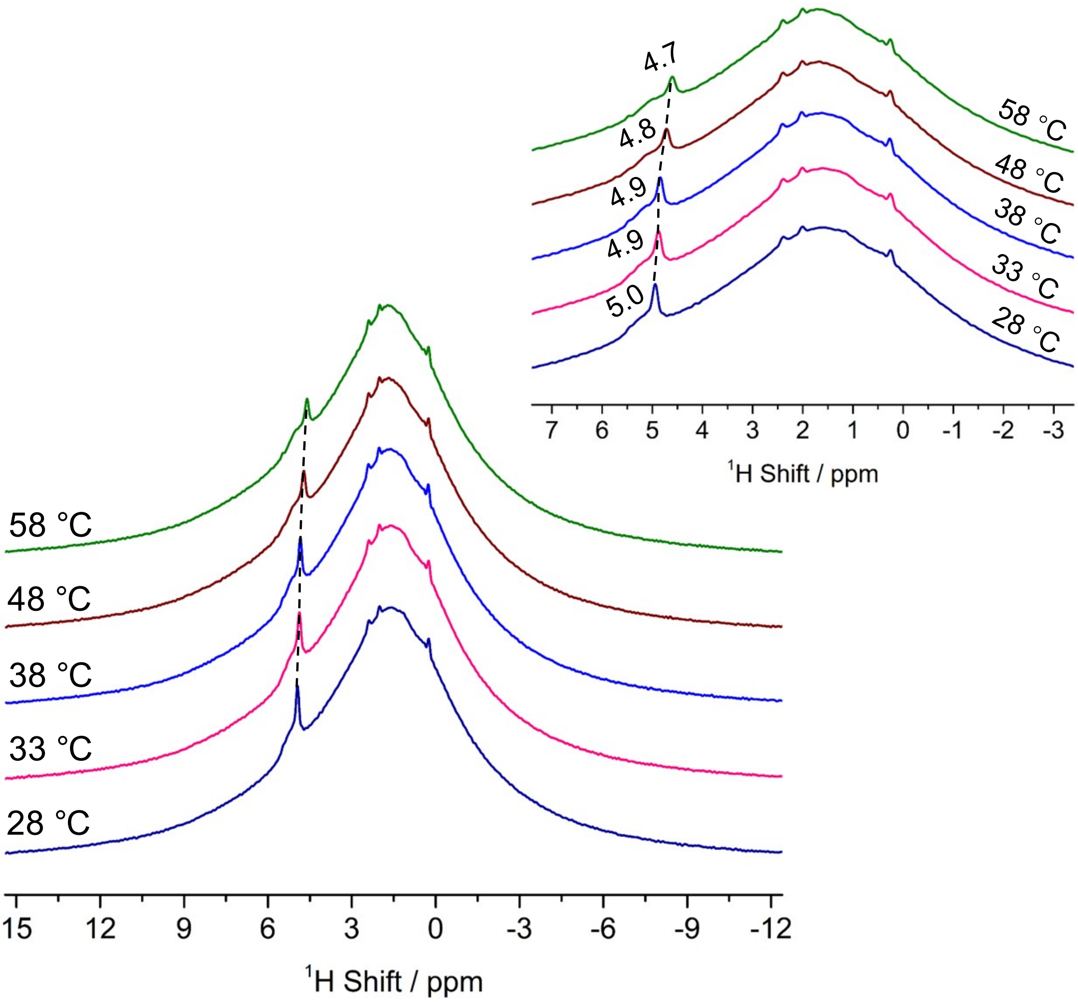

Figure S8. Variable temperature ^{1}H NMR spectra of ZnO nanoplates. Recycle delays of 5 s were used and 64 scans were collected for each NMR spectrum.

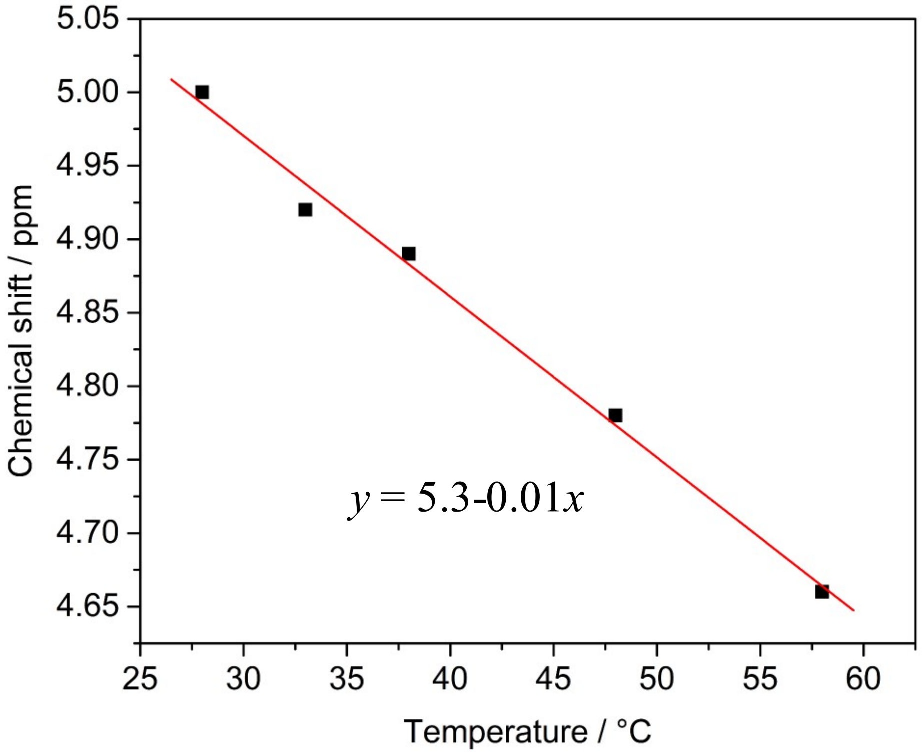

Figure S9. The chemical shifts of the high-frequency peak of ZnO nanoplates as a function of probe temperature.

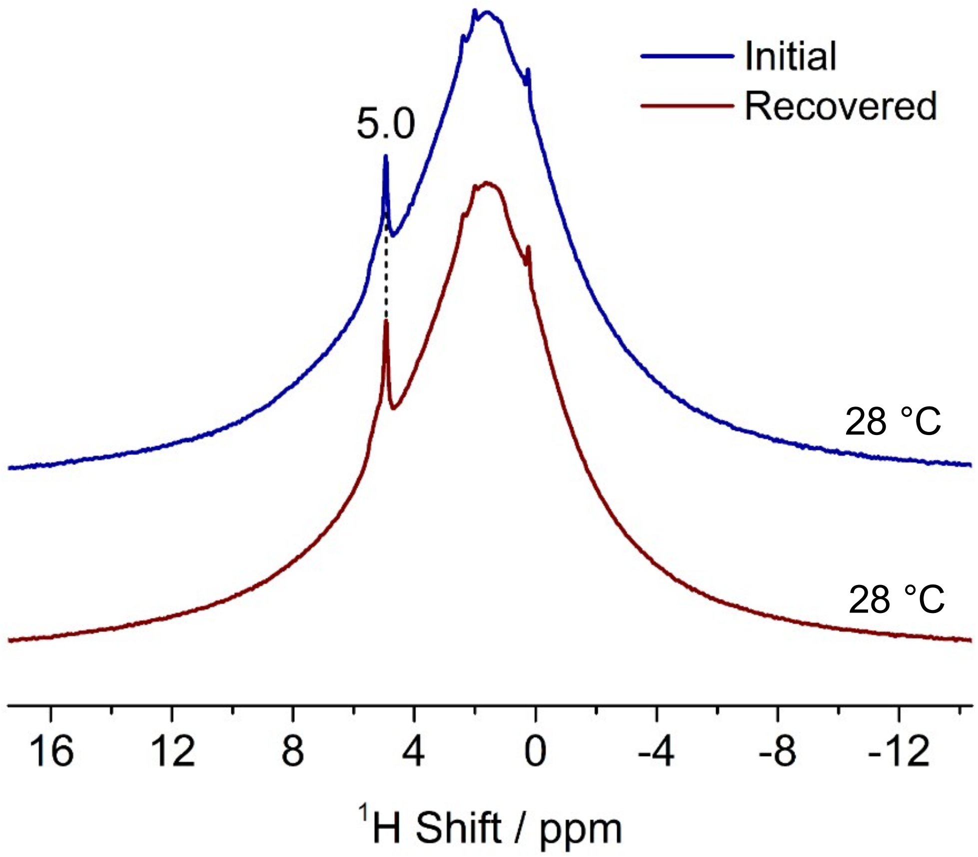

Figure S10. ^{1}H NMR spectra of ZnO nanoplates. ^{1}H NMR spectrum was first measured at 28 °C, and then exposing to different probe temperatures from 28 to 58 °C, as shown in Figure S8. Subsequently, the probe was cooled to its original temperature of 28 °C and the corresponding ^{1}H NMR spectrum of ZnO nanoplates was recorded again. Recycle delays of 5 s were used and 64 scans were collected for each NMR spectrum.

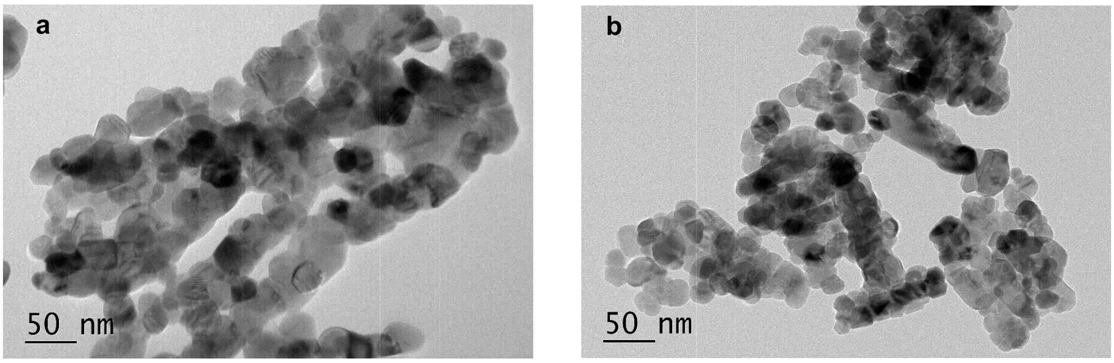

Figure S11. TEM images of ZnO nanoplates. (a) Initial samples with calcination. (b) ZnO samples without calcination were first exposed to water vapor for two weeks and then calcined at 300 °C.

References

1 C. P. Grey and A. J. Vega, *J. Am. Chem. Soc.*, 1995, **117**, 8232–8242.

2 B. T. Song, Y. H. Li, X.-P. Wu, F. Wang, M. Lin, Y. H. Sun, A.-P. Jia, X. Ning, L. Jin, X. K. Ke, Z. W. Yu, G. Yang, W. H. Hou, W. P. Ding, X.-Q. Gong and L. M. Peng, *J. Am. Chem. Soc.*, 2022, **144**, 23340−23351.