Electronic Supplementary Material (ESI) for Nanoscale.

Highly electron-deficient ultrathin Co nanosheets supported on mesoporous Cr_2O_3 for catalytic hydrogen evolution from ammonia borane

Jin Song[a] and Fenglong Wu*[a]

[a] Department of Chemical and Environmental Engineering, Hetao College, Bayan Nur 015000, China

E-mail: wufenglong1983@126.com

Calculation method of TOF value

The TOF value is calculated by the following equation.

$$TOF = \frac{3n_{NH_3BH_3}}{n_{metal}t}$$

In this equation, n_{metal} means the total molar amount of Co species on the surface of Cr_2O_3, t means the hydrogen evolution time, and $n_{NH_3BH_3}$ means the molar amount of NH_3BH_3 introduced in the system**.**

Support preparation

Preparation Of C_3N_4: 4.99g urea were milled into powder and placed in muffle furnace 500 °C for 2h.

Preparation Of WO_3: WO_3 nanoparticles were prepared based on literature.[1] Specifically, WCl_6 (1.029g) and hexamethylenetetramine (0.1728g) was dissolved in 30mL n-butanol solution. After that the above solution was placed into autoclave and kept at 160 °C for 24 h. The obtained samples were washed with high purity water and absolute ethanol for several times and then heated at 70 °C for 10 h. Finally, the samples were calcined in muffle furnace at 500 °C for 2 h.

Preparation Of MoO_3: 0.99g ammonium molybdate tetrahydrate ($H_2MoN_6O_{24}$ $4H_2O$) were placed in muffle furnace 600 °C for 2h.

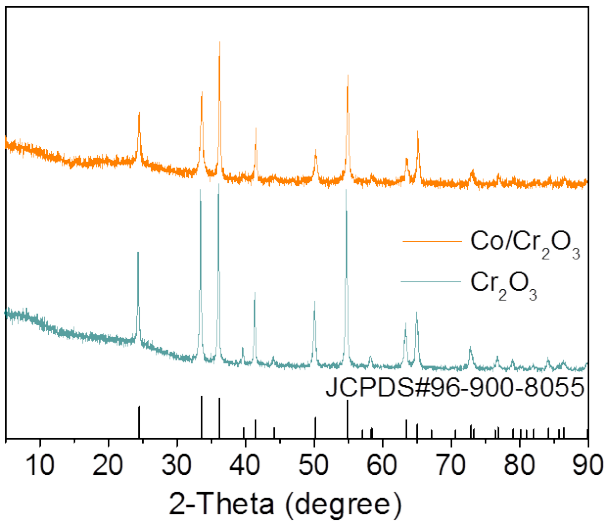

Fig. S1 XRD patterns of samples.

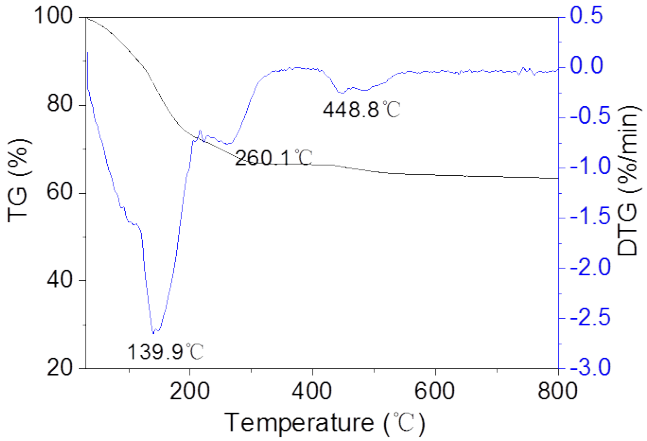

Fig. S2 TGA and DTG of the precursor sample of mesoporous Cr_2O_3.

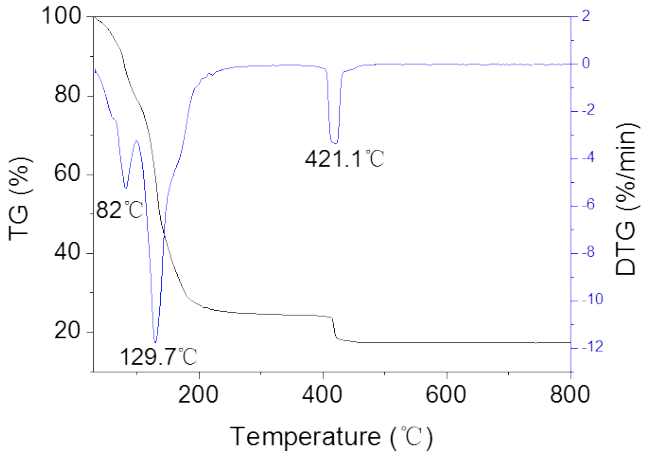

Fig. S3 TGA and DTG of the precursor sample of Cr_2O_3.

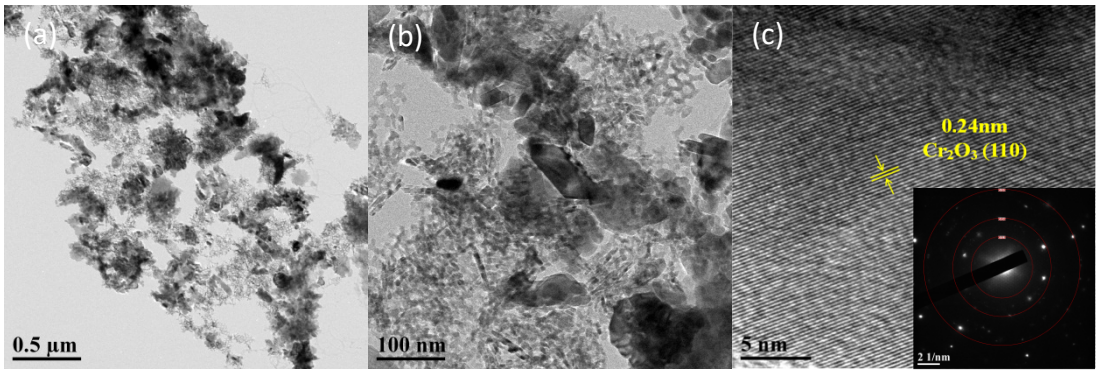

Fig S4 TEM and HRTEM images of Cr_2O_3.

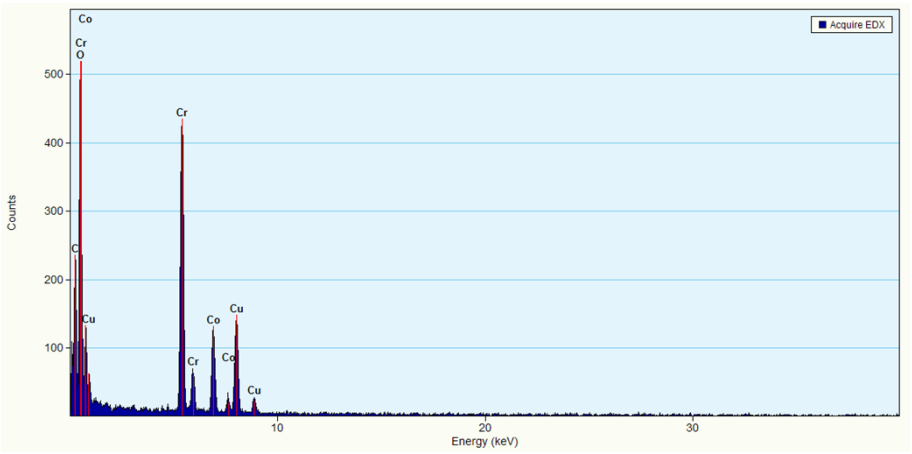

Fig. S5 EDS of Co/Cr_2O_3.

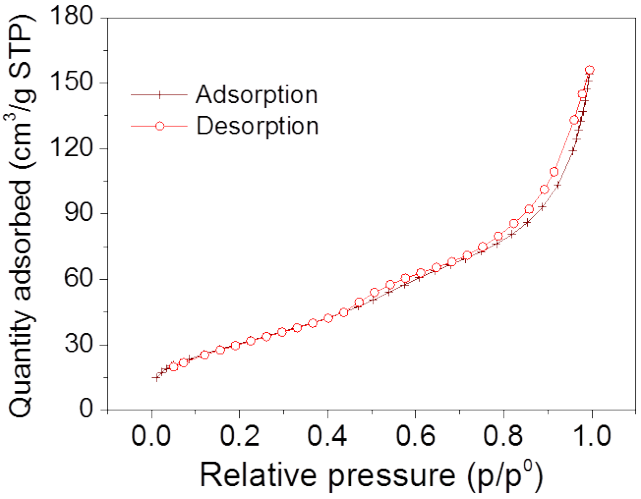

Fig. S6 N_2 adsorption-desorption isotherms of Co/Cr_2O_3.

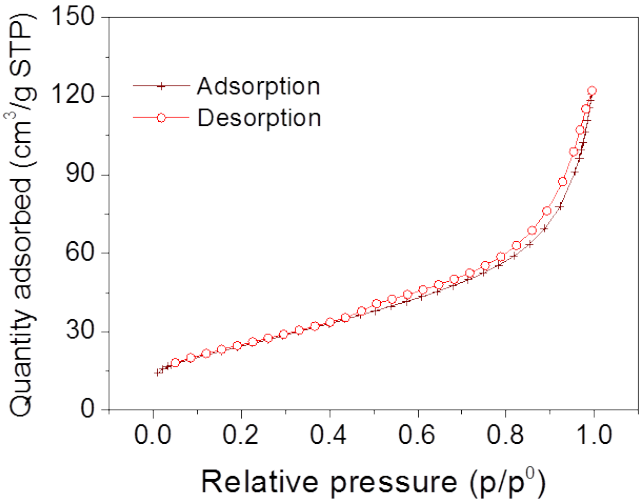

Fig. S7 N_2 adsorption-desorption isotherms of mesoporous Cr_2O_3.

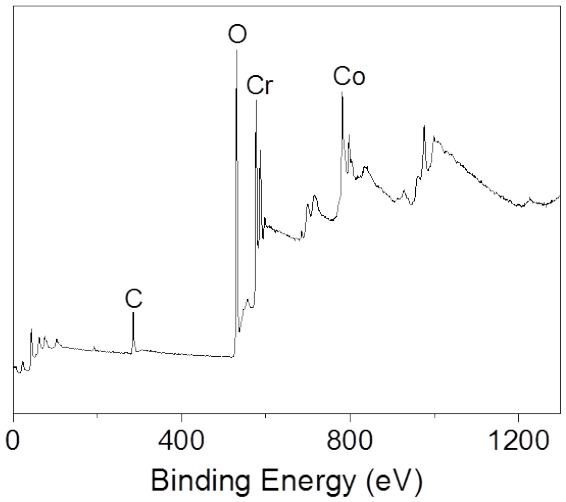

Fig. S8 XPS spectra for Co/Cr_2O_3.

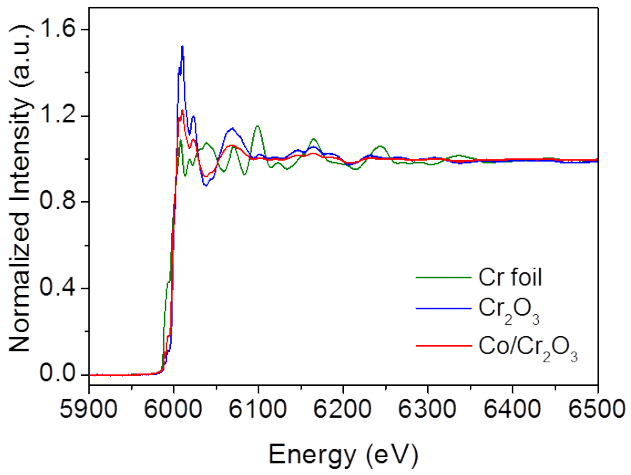

Fig. S9 Normalized XANES spectra of Cr foil, Cr_2O_3, and Co/Cr_2O_3 at the Cr K-edge.

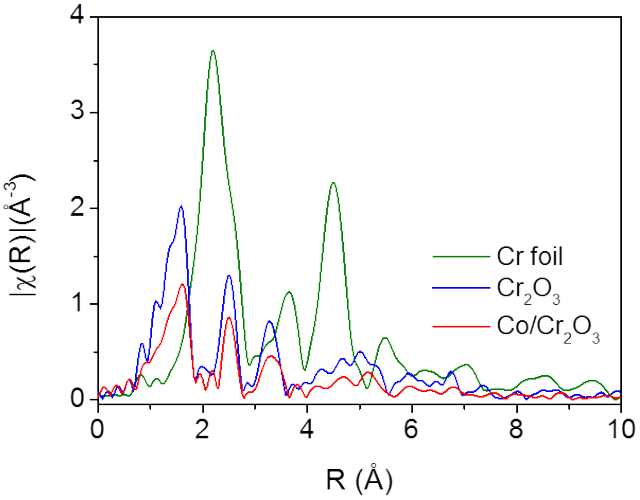

Fig. S10 Fourier transform EXAFS spectra of Cr foil, Cr_2O_3, and Co/Cr_2O_3 at the Cr K-edge.

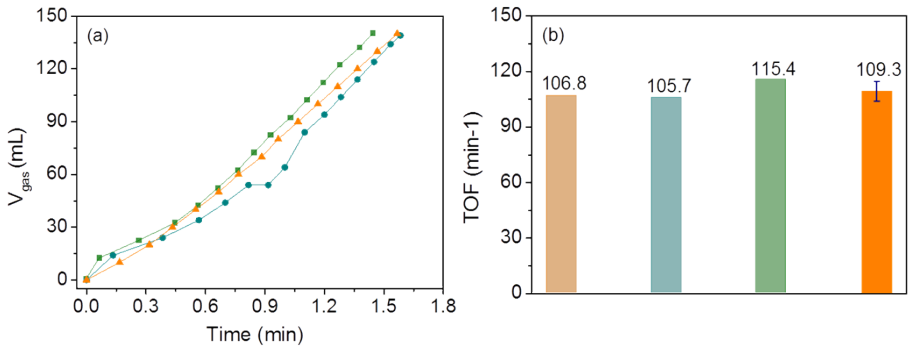

Fig. S11 Plots of time versus volume of H_2 evolution from NH_3BH_3 in the aqueous solution over Co/Cr_2O_3 under visible light irradiation, (b) TOF value and corresponding error bar.

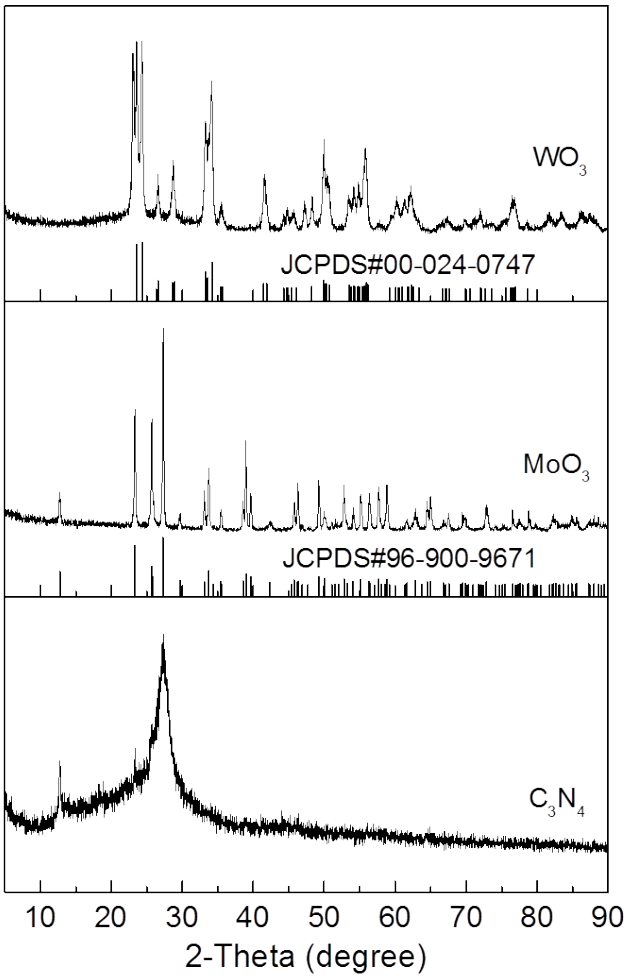

Fig. S12 XRD patterns of samples.

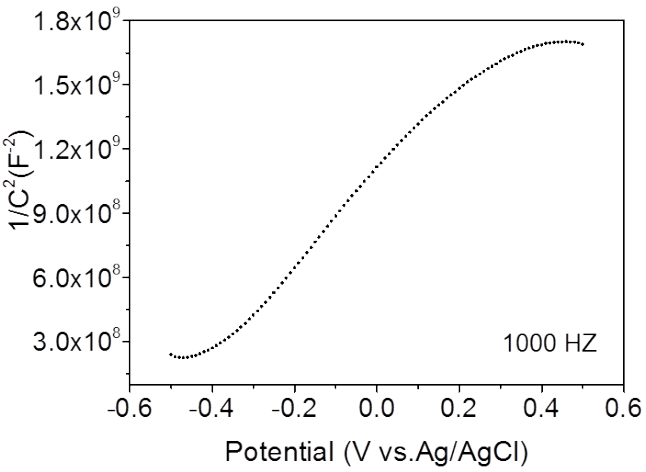

Fig. S13 Mott-Schottky plots of C_3N_4.

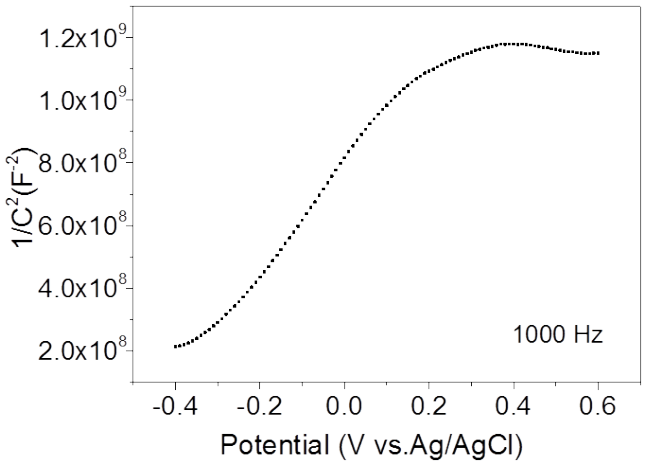

Fig. S14 Mott-Schottky plots of MoO_3.

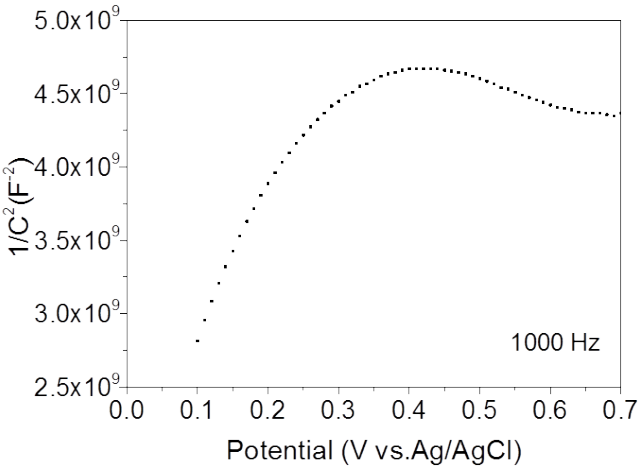

Fig. S15 Mott-Schottky plots of WO_3.

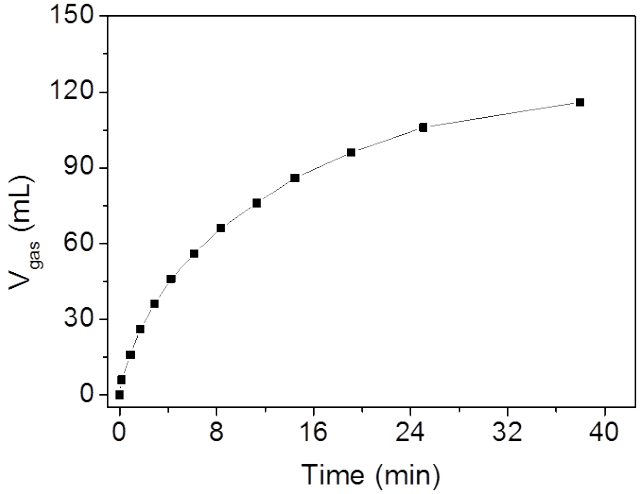

Fig. S16 Plots of time versus volume of H_2 evolution from NH_3BH_3 in the aqueous solution over Co/MoO_3 in dark.

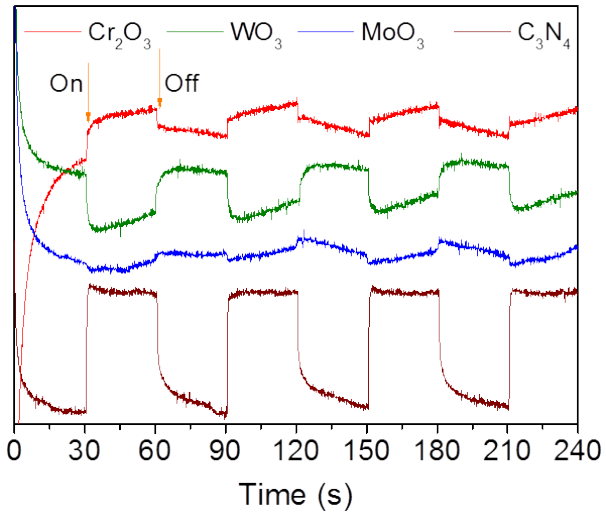

Fig. S17 Profiles of time versus transient photocurrent density of the samples.

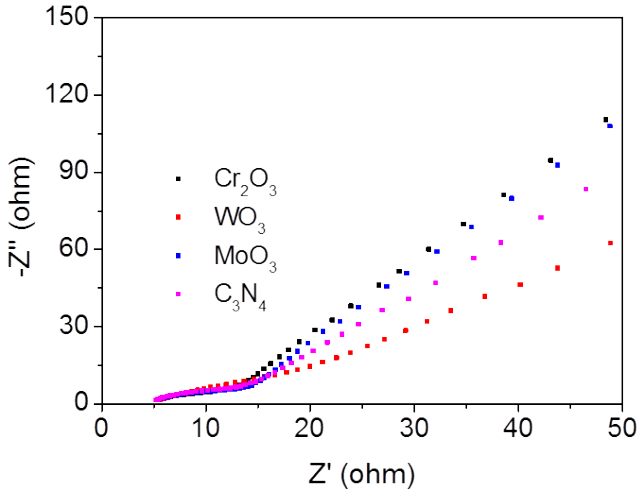

Fig. S18 EIS Nyquist plots of samples.

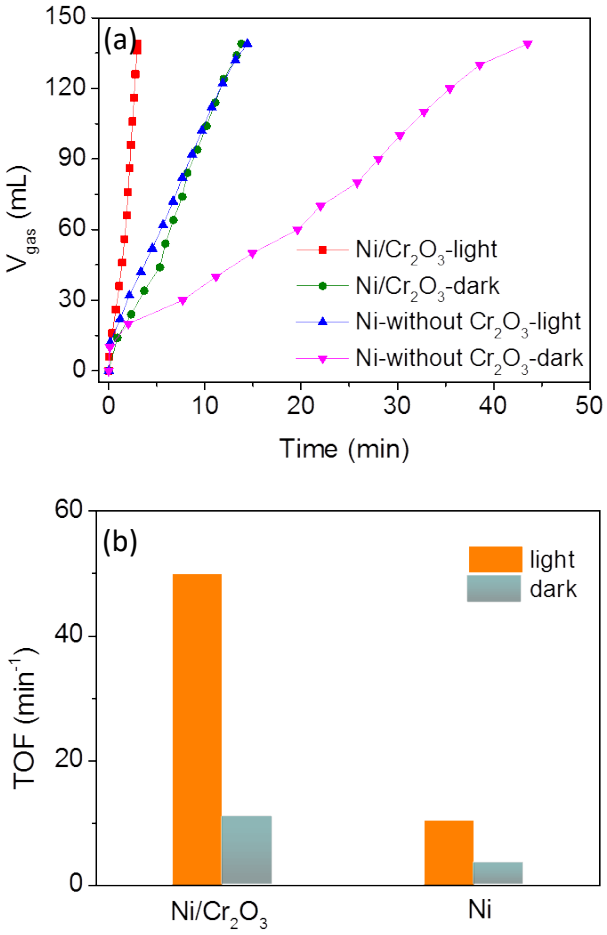

Fig. S19 (a) Plots of time versus volume of H_2 evolution from NH_3BH_3 in the aqueous solution over Ni-based catalysts in dark and under visible light irradiation, (b) corresponding TOF value.

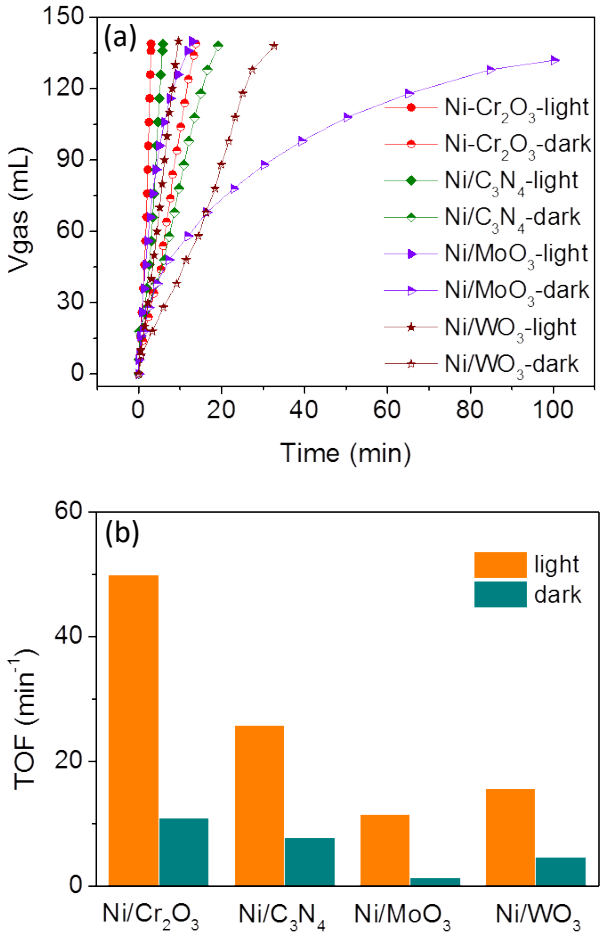

Fig. S20 (a) Plots of time versus volume of H_2 evolution from NH_3BH_3 in the aqueous solution over Ni-based catalysts with photoactive semiconductor as support in dark and under visible light irradiation, (b) corresponding TOF value.

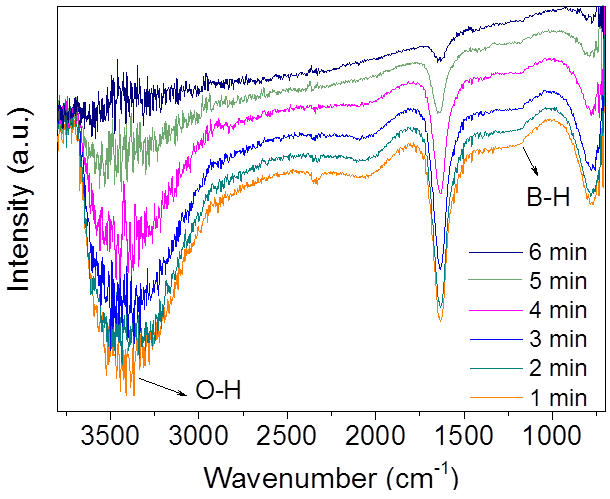

Fig. S21 The time evolutions of the DRIFTS spectra of NH_3BH_3 hydrolysis over Co/Cr_2O_3 catalyst

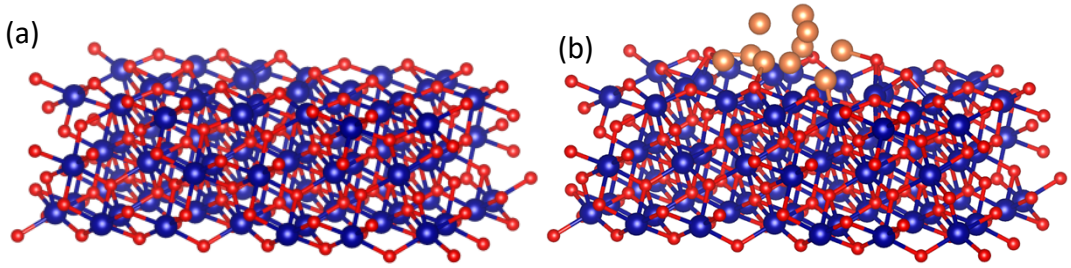

Fig. S22 Clean surface of (a) Cr_2O_3 and (b) Co/Cr_2O_3.

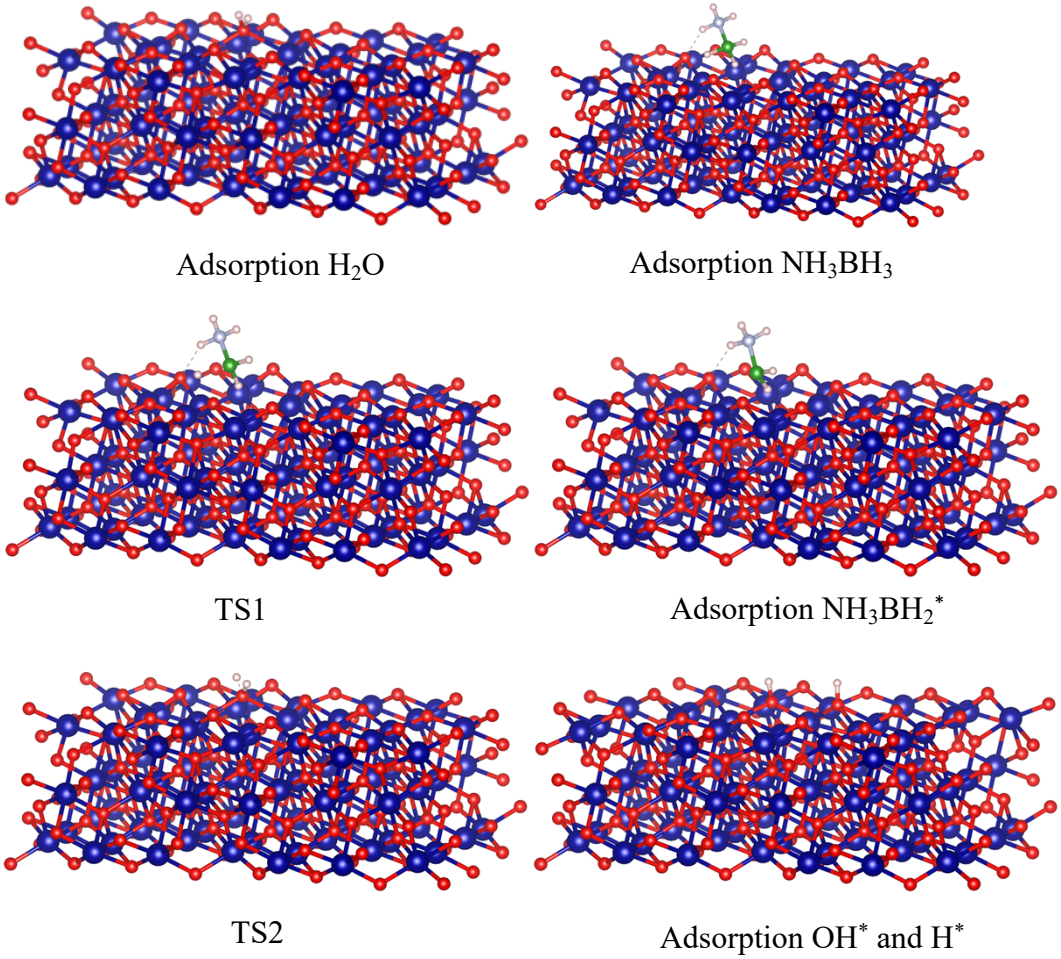

Fig. S23 DFT calculated intermediate structures for the reactions of NH_3BH_3 hydrolysis on Co/Cr_2O_3.

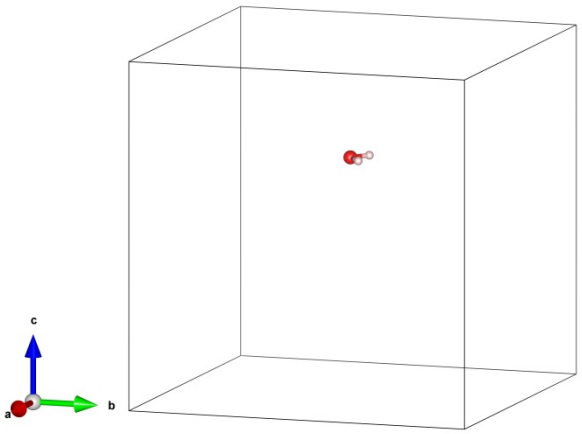

Fig. S24 Single unit cell of H_2O

References

1 X. Wang, F. Chen, M. Yang, L. Guo, N. Xie, X. Kou, Y. Song, Q. Wang, Y. Sun and G. Lu, *Sensor. Actuat. B: Chem.*, 2019, **289**, 195–206.