Supporting Information for: Zirconium Modification Promotes Catalytic Activity of a Single-Site Cobalt Heterogeneous Catalyst for Propane Dehydrogenation

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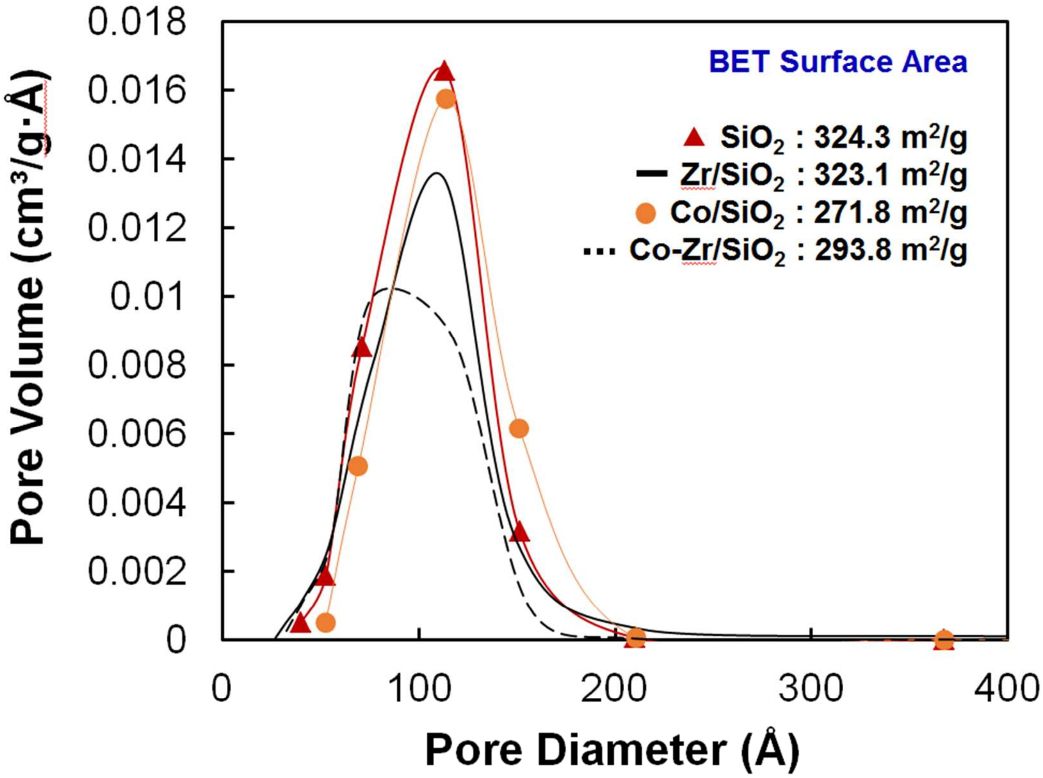


Figure S1. BET surface areas and BJH pore size distributions of SiO_2, Zr/SiO_2, Co/SiO_2 and Co-Zr/SiO_2

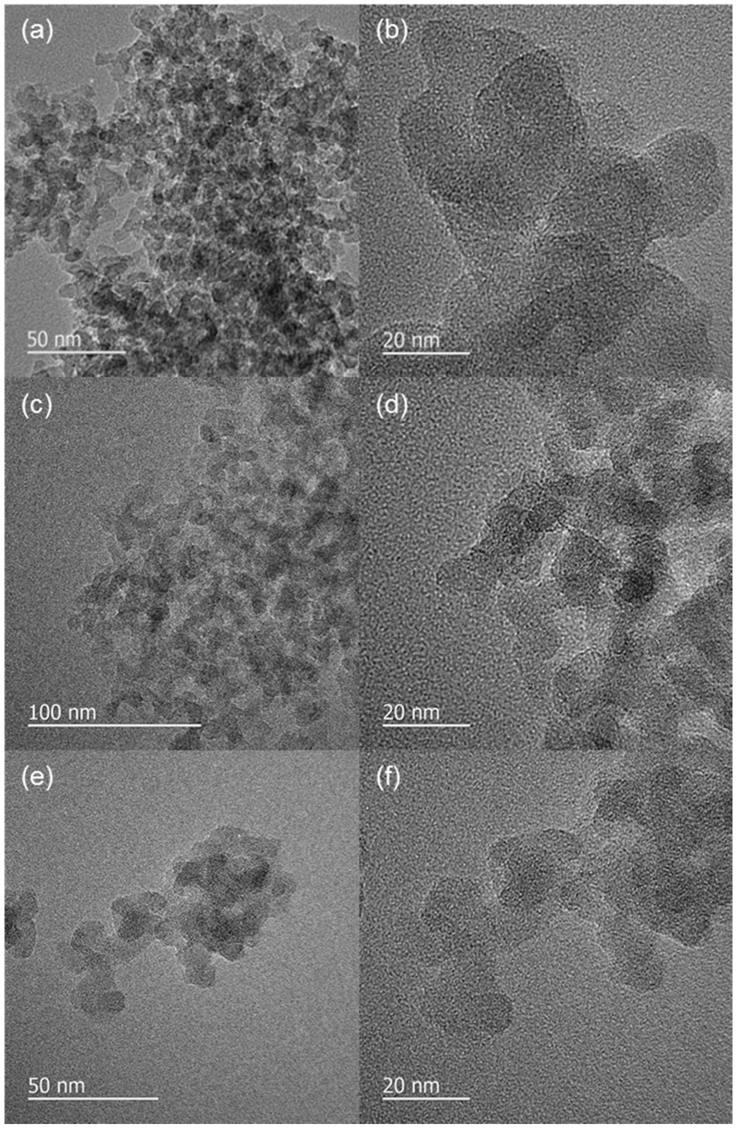


Figure S2. TEM images of (a, b) Zr/SiO_2, (c,d) Co/SiO_2 and (e,f) $Co\text{-}Zr/SiO_2$

The particle size and morphology of the as-prepared catalyst materials was examined by TEM and are shown in Figure S2. The TEM images were taken at multiple random locations to improve the consistency of the analysis. The images in Figure S2 (a, b) show Zr/SiO_2 support with no large clusters of ZrO_x from the initial synthesis. Similarly, addition of cobalt onto SiO_2 and Zr/SiO_2 supports retains the well-dispersed surface sites. As it can be seen in Figure S2 (c, d) (e, f) neither the Co/SiO_2 nor the $Co\text{-}Zr/SiO_2$ samples indicate formation of nanoparticles to the limit of the TEM resolution. TEM-EDX analysis also shows well-dispersed Zr and Co.

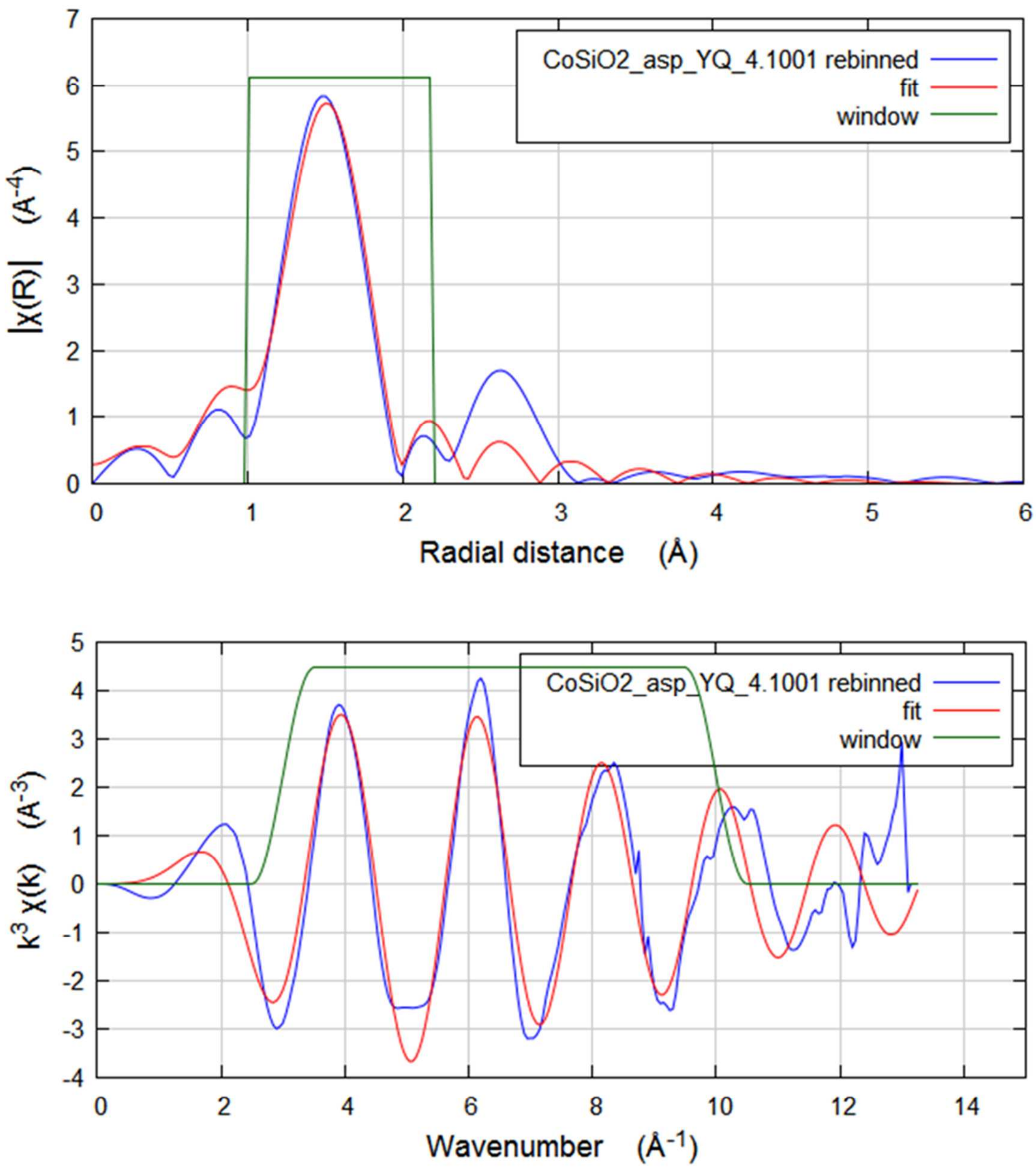


Figure S3. EXAFS data and fit for Co/SiO_2 as-prepared in (1) *R*-space (top) and (2) *k*-space (bottom).

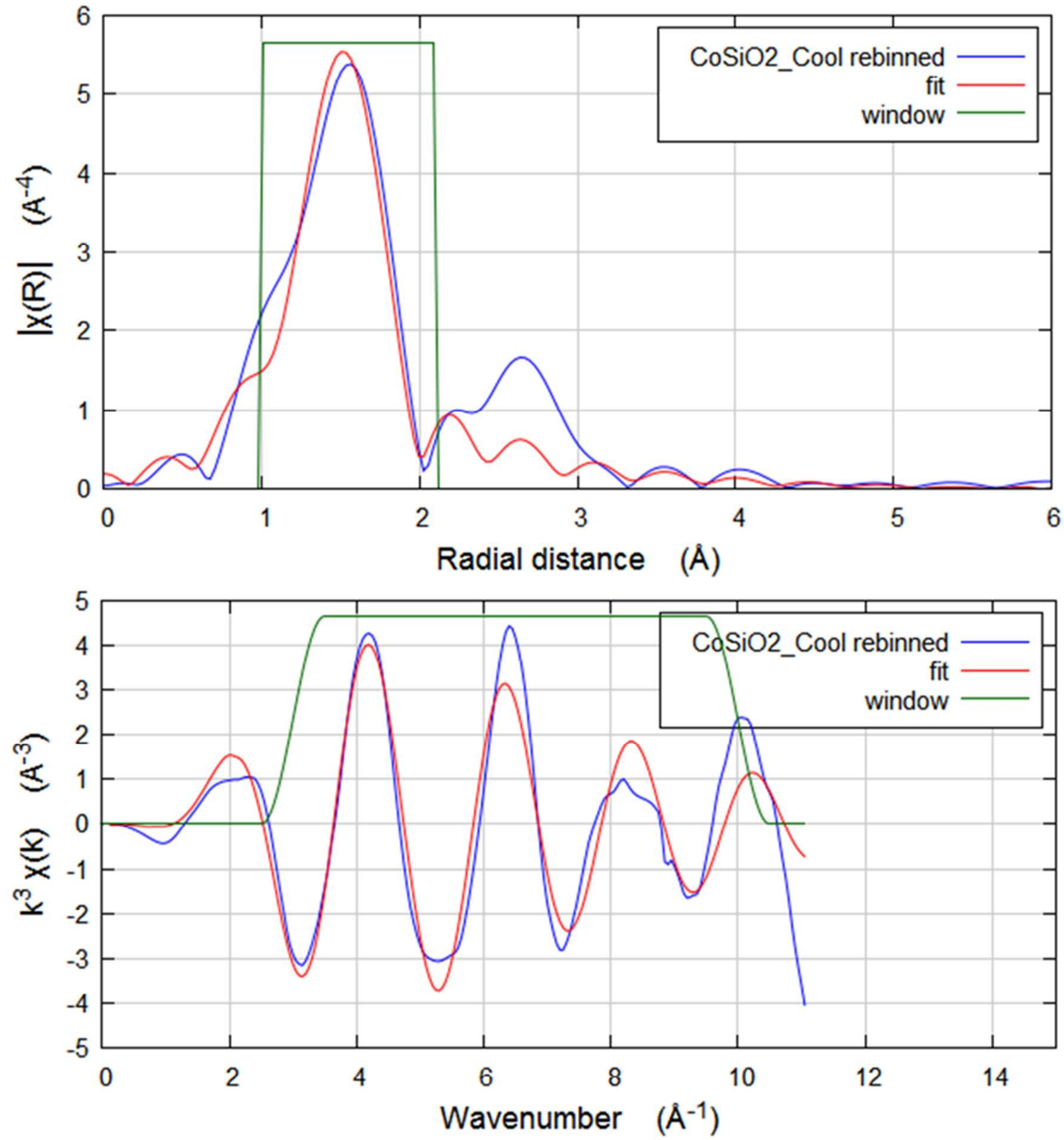
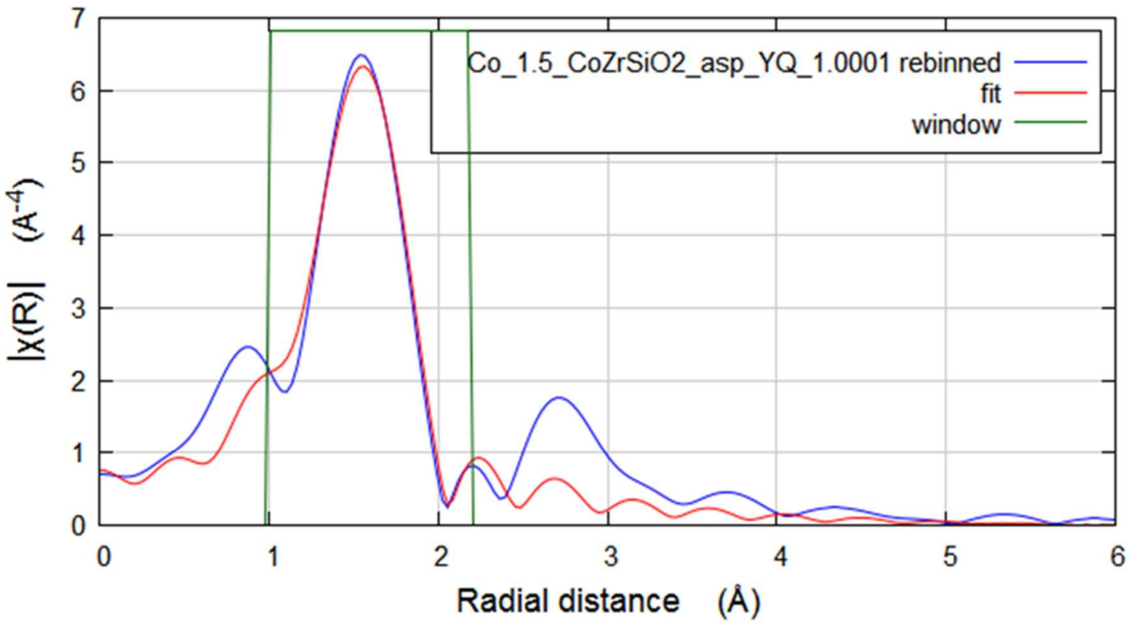


Figure S4. EXAFS data and fit for Co/SiO_2 cooled down to room temperature after catalysis in (1) *R*-space (top) and (2) *k*-space (bottom).



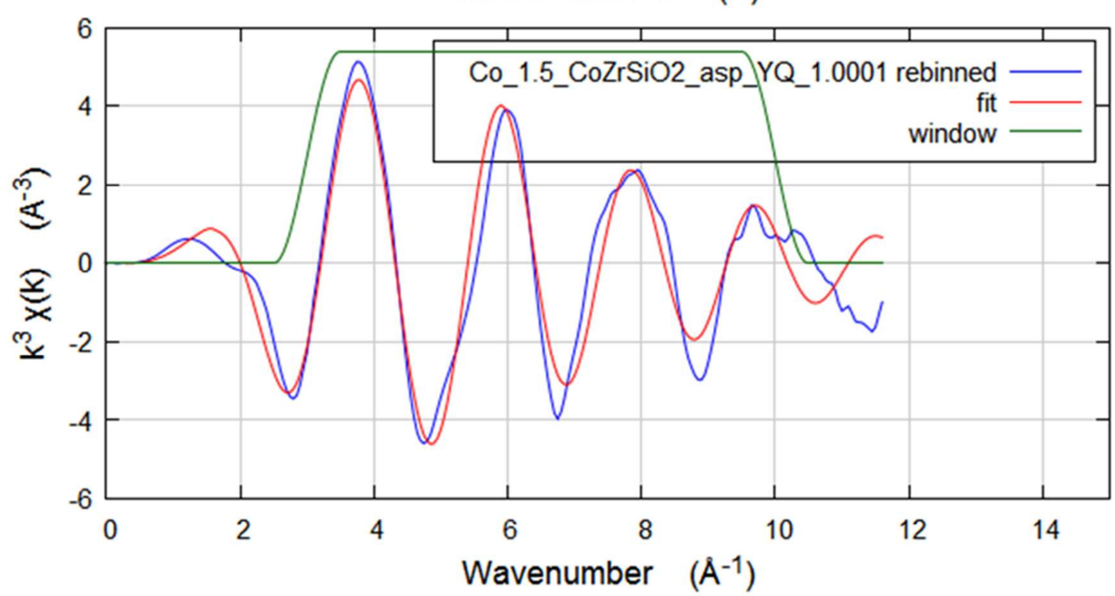


Figure S5. EXAFS data and fit for Co-Zr/SiO_2 as-prepared in (1) *R*-space (top) and (2) *k*-space (bottom).

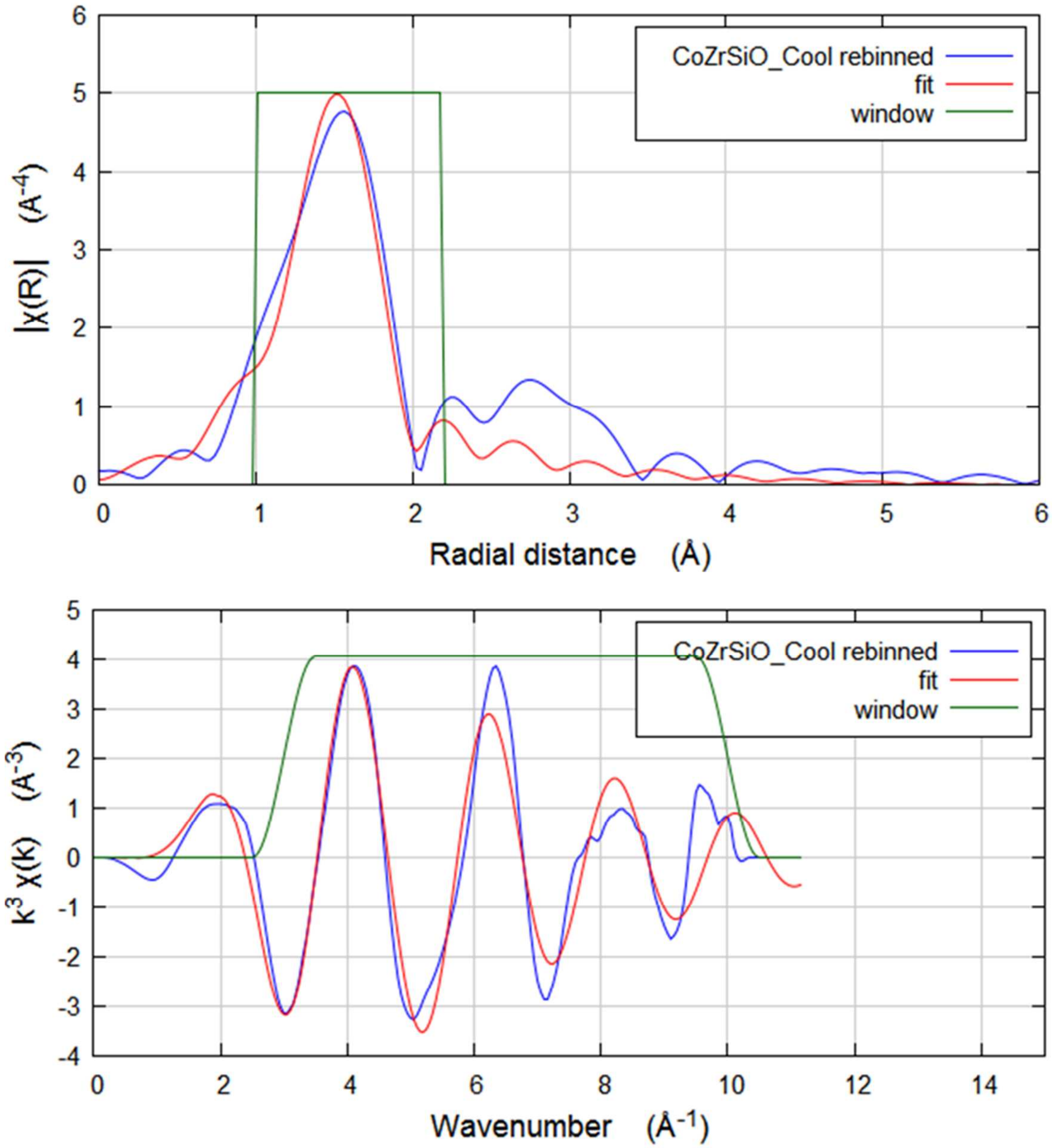


Figure S6. EXAFS data and fit for Co-Zr/SiO_2 cooled down to room temperature after catalysis in (1) *R*-space (top) and (2) *k*-space (bottom).

Synthesis of Co/ZrO_2 catalyst

Cobalt was grafted onto ZrO_2 via incipient wetness impregnation (IWI) using $Co(NH_3)_6Cl_3$. ZrO_2 was dried at 200 °C for 4h to establish a reproducible weight and hydration level. 0.1362g $Co(NH_3)_6Cl_3$ was dissolved in to 1mL of DI water, then $Co(NH_3)_6Cl_3$ solution was dropped on ZrO_2 (2.0 g) and dried at 120 °C for 2h Then the sample was calcined in air to 300 °C for 4h and resulting cobalt loading was 1.5%.

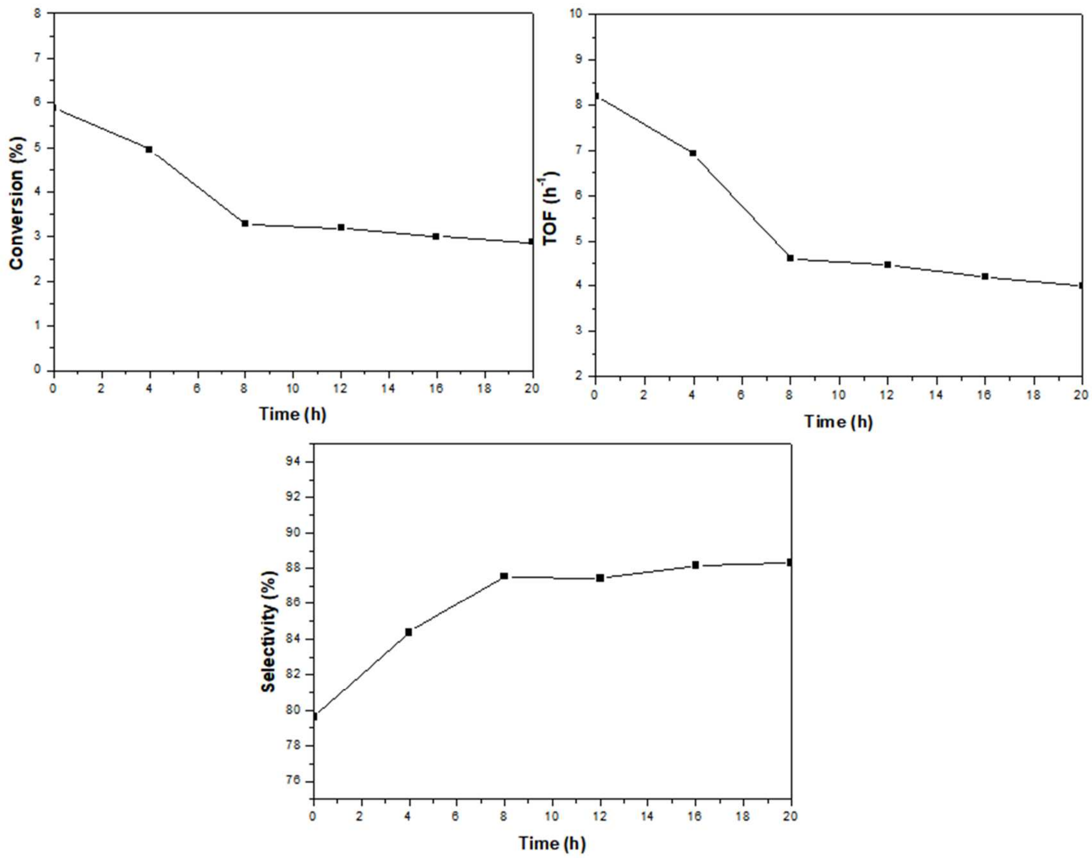


Figure S7. Propane dehydrogenation reactivity and selectivity performed at 550 °C, propane (3% in argon) flow rate is 20 mL/min, using Co/ZrO_2 catalyst.