Supporting Information for

Participation of Interfacial Hydroxyl Groups in the Water-Gas Shift Reaction over Au/MgO Catalysts

Yanran Cui[a§], Zhenglong Li[a,b§], Zhijian Zhao[a], Viktor J. Cybulskis[a], Kaiwalya D. Sabnis[a], Chang Wan Han[c], Volkan Ortalan[c], William F. Schneider[d], Jeffrey Greeley[a], W. Nicholas Delgass[a§§] and Fabio H. Ribeiro[a§§]

[a] *Charles D. Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN 47907(USA)*

[b] *Energy and Transportation Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831 (USA)*

[c] *School of Materials Engineering, Purdue University, West Lafayette, IN 47907(USA)*

[d] *Department of Chemical and Biomolecular Engineering, University of Notre Dame, Notre Dame, IN 46556 (USA)*

§ Co-first authors, §§ Co-corresponding authors

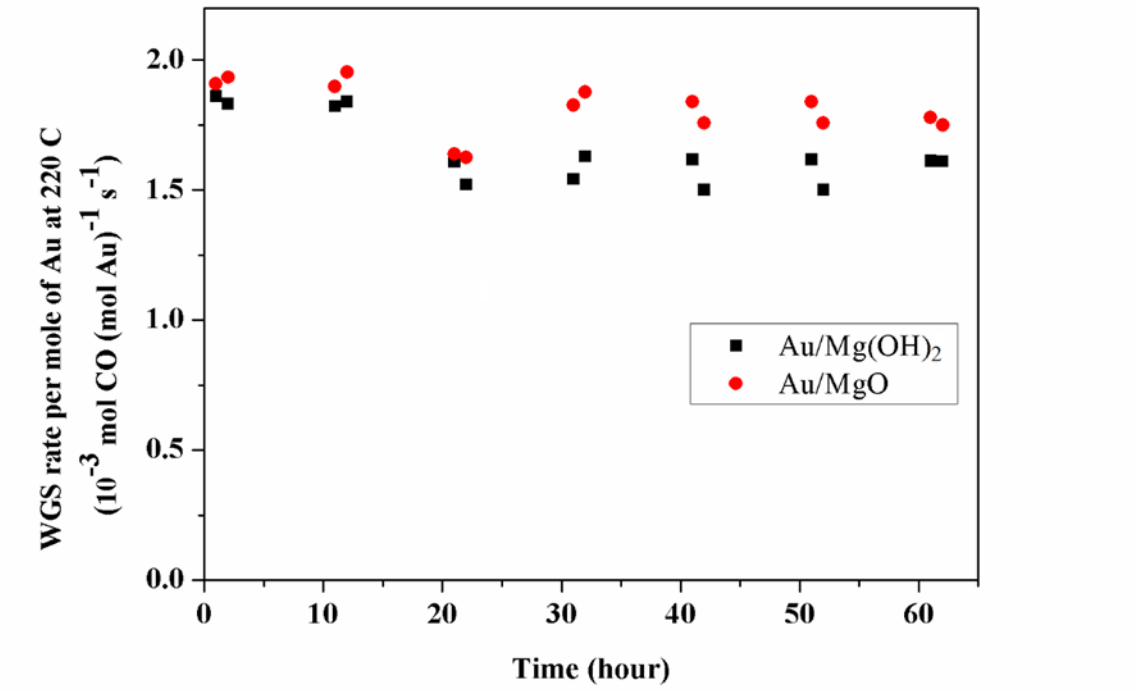
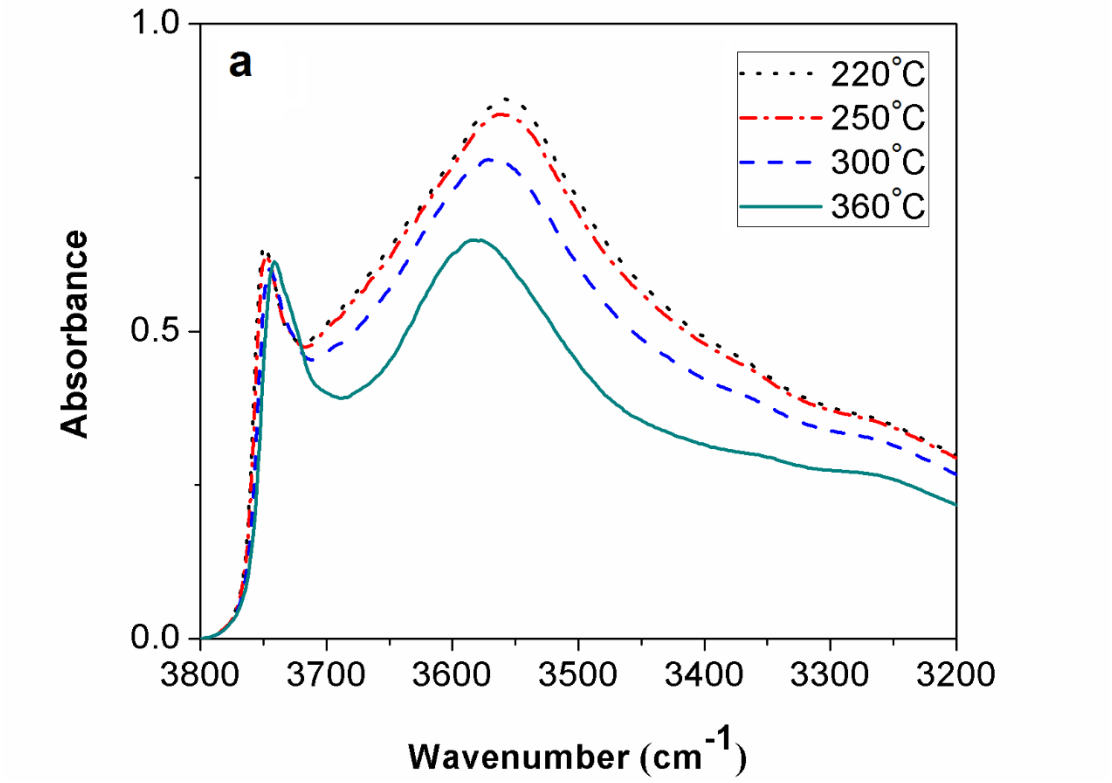


Figure S1. Deactivation plot during the measurement of WGS kinetics (standard conditions, 6.8% CO, 21.9% H_2O, 8.5% CO_2, 37.4% H_2, and balance Ar).


a
220°C
250°C
300°C
360°C
Absorbance
1.0
0.5
0.0
3800
3700
3600
3500
3400
3300
3200
Wavenumber (cm-1)

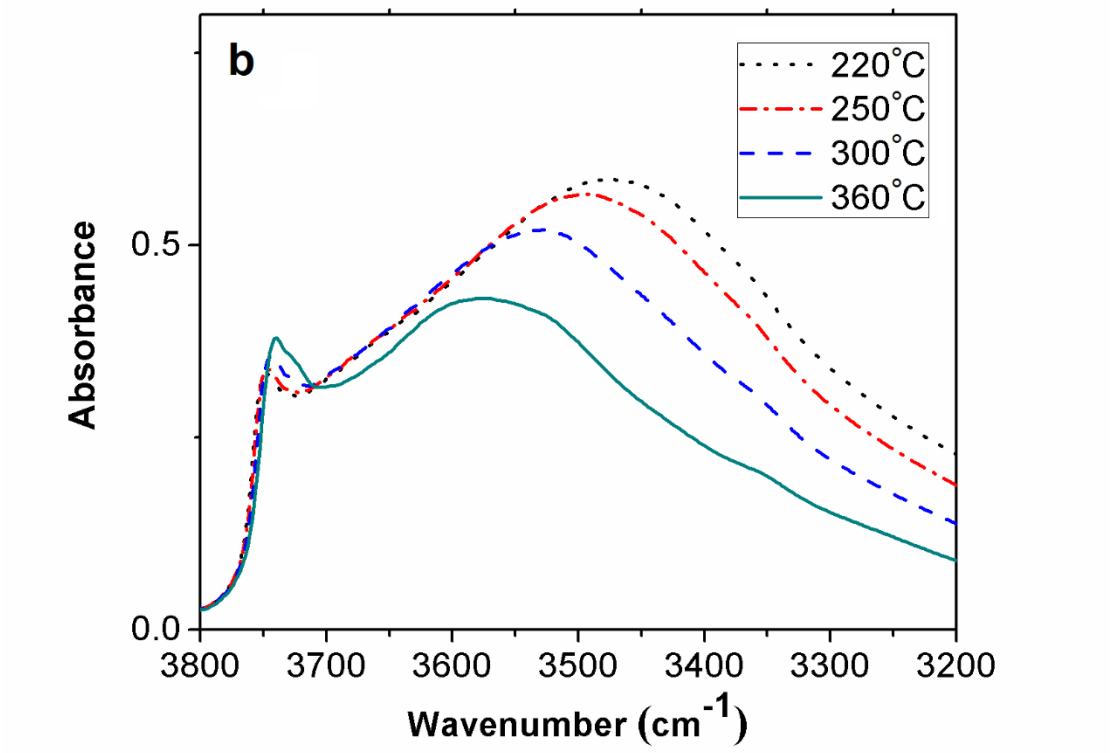

b
220°C
250°C
300°C
360°C
Absorbance
0.5
0.0
3800
3700
3600
3500
3400
3300
3200
Wavenumber (cm-1)

Figure S2. N_2 TPD (ramp rate: 5 °C min^{-1}) after exposure to 11% H_2O/N_2: a) Au/MgO b) MgO Support. Both samples were pretreated by reduction in 25% H_2/N_2 at 150 °C for 2 hours (flow rate: 50 ml min^{-1}, ramp rate: 2 °C min^{-1}) followed by annealing in N_2 at 400 °C for 2 hours (flow rate: 50 ml min^{-1}, ramp rate: 5 °C min^{-1}).

Table S1. Simulated relative WGS rates by manually tuned (D-OD)*# binding energy

ΔBE^a / eV	0	+0.02	+0.03	+0.04
r_H/r_D	1.02	1.42	1.77	2.22

[a]: Manually tuned (D-OD)*# binding energy (eV). Positive number indicates weakening (D-OD)*# binding strength.