Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

High Coverage Adsorption and Co-Adsorption of CO and H_2 on Ru(0001) from DFT and Thermodynamics

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Figure S1. Stepwise CO adsorption structures and energies (ΔE_{ads}) on Ru(0001) using the PBE functional (surface Ru/blue; C/black; O/red).

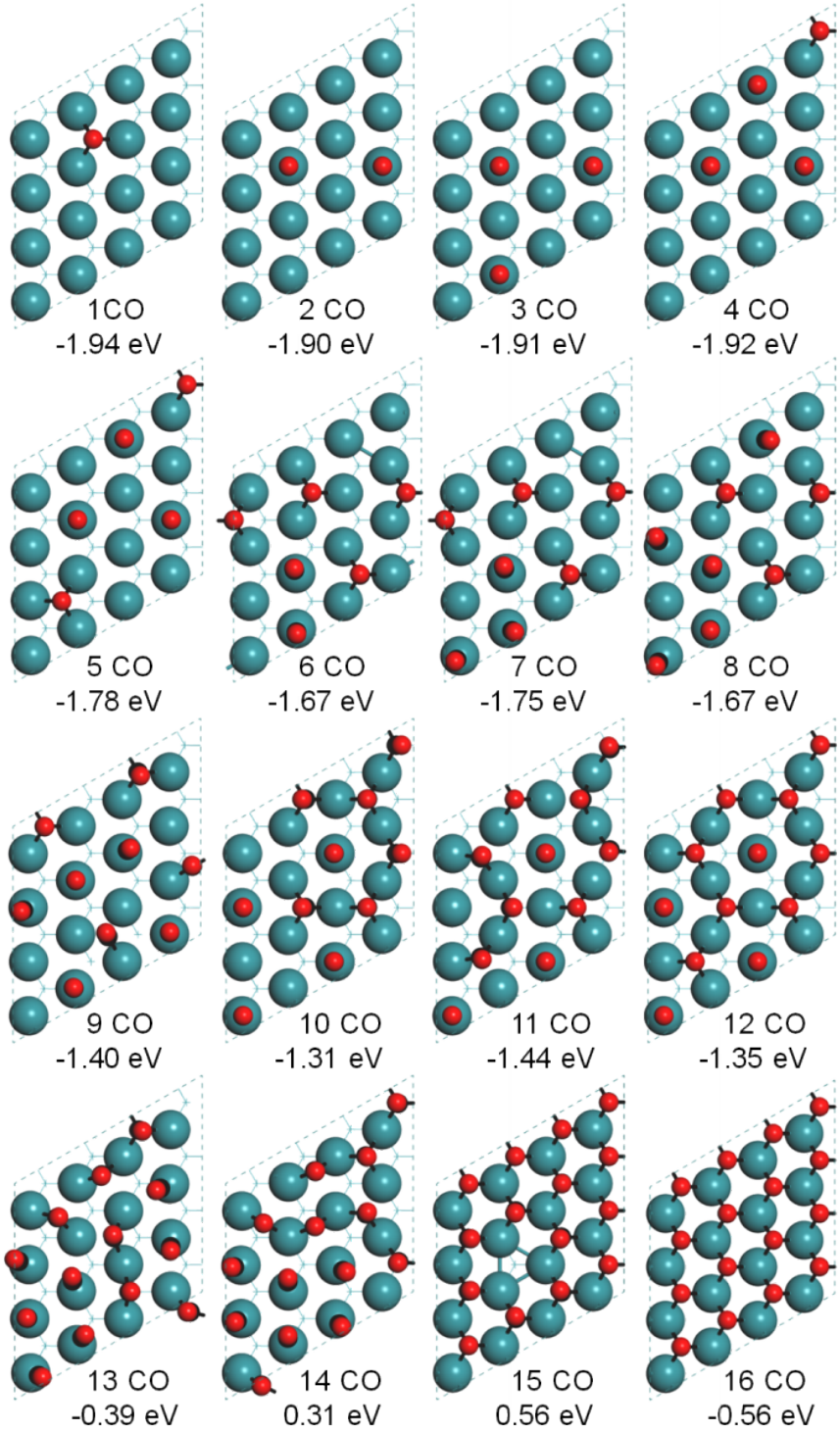

Figure S2: 10CO and 14CO adsorption structures and energies (ΔE_{ads}) on Ru(0001) using the PBE and PBE+D3

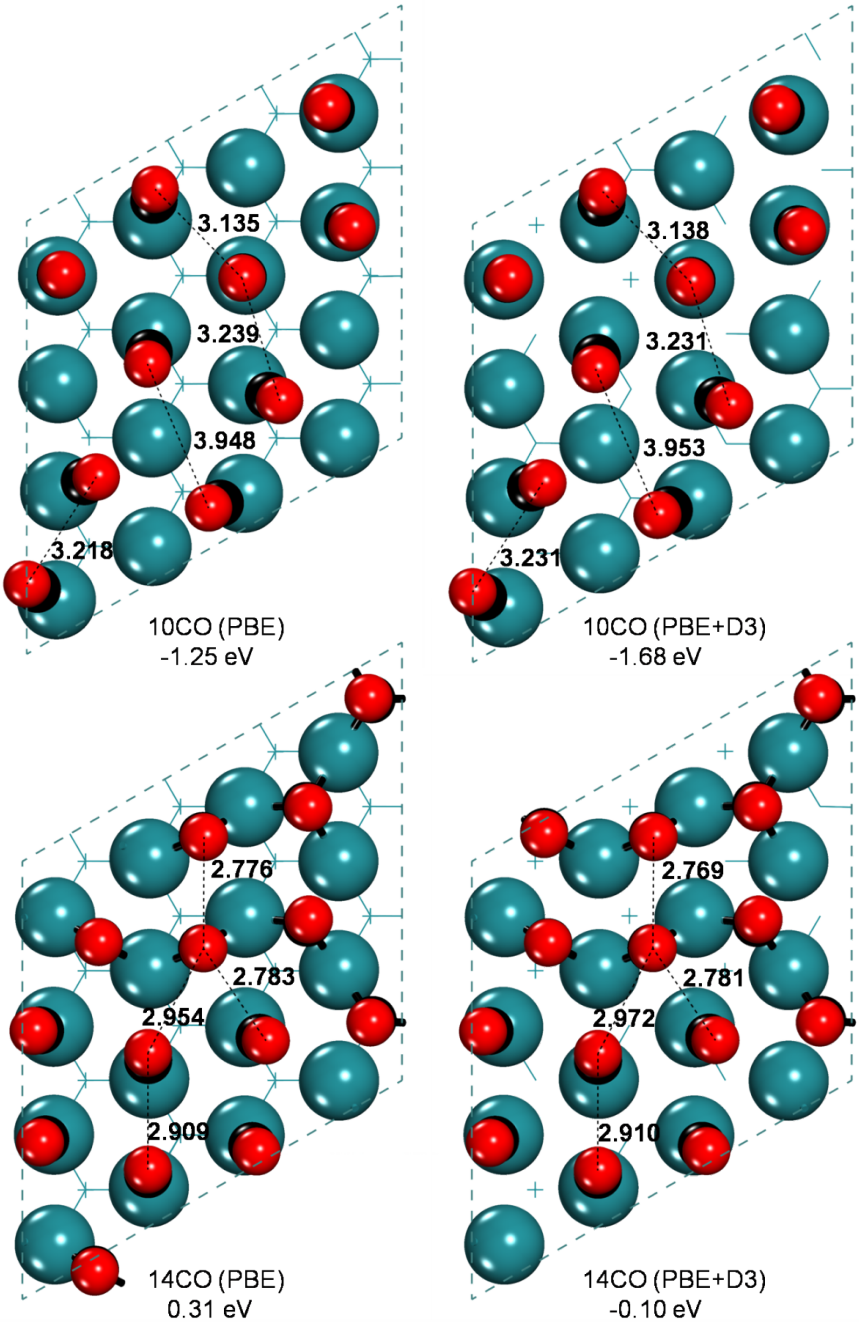

Figure S3. Stepwise H_2 adsorption structures and energies (ΔE_{ads}) on nCO pre-covered Ru(0001) (n =1-8, surface Ru/blue; C/black; O/red; H/yellow).

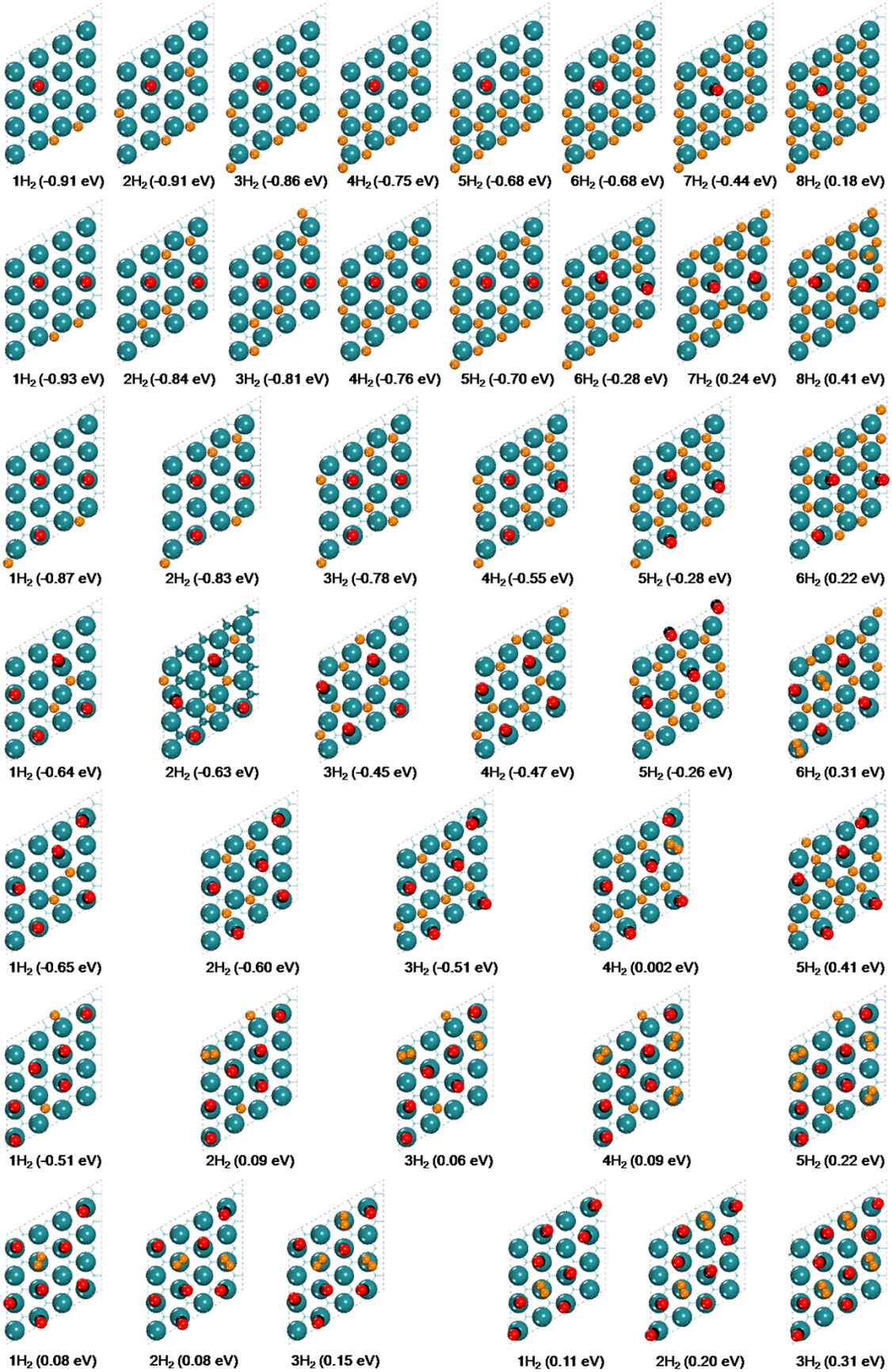

Figure S4: Dependence of surface Gibbs free energy (ΔG) and H_2 on temperature at $p_{H2}/p^0 = 1\times10^{-13}$

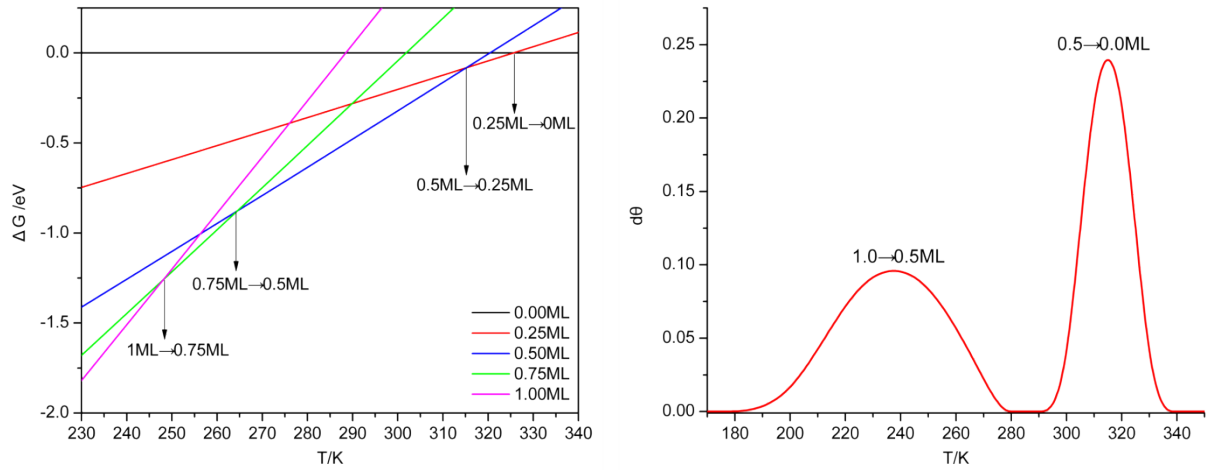

Table S1. Stepwise CO adsorption energies (E_{ads}, eV) including D3 corrections at different coverage

ML	E_{ads}[a]	E_{ads}[b]
0.06	-2.20	-2.38
0.13	-2.20	-2.37
0.19	-2.18	-2.25
0.25	-2.22	-2.14
0.31	-2.04	-2.40
0.38	-2.13	-2.01
0.44	-2.11	-2.46
0.5	-1.84	-2.21
0.56	-1.86	-2.40
0.63	-1.70	-2.06
0.69	-2.03	-2.43
0.75	-1.82	-2.05
0.81	-0.96	-1.58
0.88	-0.11	-0.52

(a) Derived from D3 single-point energy calculations on the PBE optimized structures in parenthesis.

(b) Derived from D3 single-point energy calculations on the RPBE optimized structures in parenthesis.